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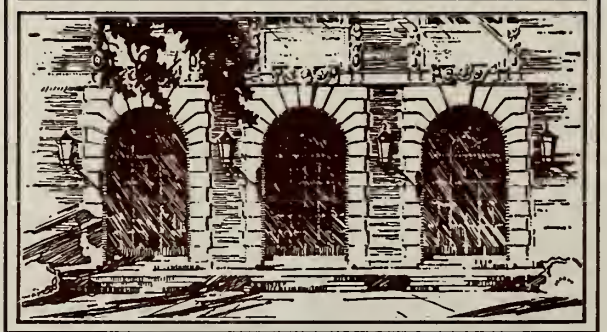

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MONTE CARLO SIMULATION OF NONLINEAR RADIATION INDUCED PLASMAS

by

Benjamin Shaw-hu Wang

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MONTE CARLO SIMULATION OF NONLINEAR RADIATION INDUCED PLASMAS

BY

BENJAMIN SHAW-hu WANG
B.S., National Taiwan University, 1960
M.S., University of Missouri (Rolla), 1964

THESIS

Submitted in partial fulfillment of the requirements
for the degree of Doctor of Philosophy in Computer Science
in the Graduate College of the
University of Illinois at Urbana-Champaign, 1972

Urbana, Illinois

MONTE CARLO SIMULATION OF NONLINEAR RADIATION INDUCED PLASMAS

Benjamin Shaw-hu Wang, Ph.D.
Department of Computer Science
University of Illinois at Urbana-Champaign, 1972

A Monte Carlo simulation model for radiation induced plasmas with nonlinear properties due to recombination has been developed, employing a piecewise linearized predict-correct iterative technique. Several important variance reduction techniques have been developed and incorporated into the model, including an antithetic variates technique (negatively correlated variates) which has proven to be most useful. This approach is especially efficient for plasma systems with inhomogeneous media, multidimensions, and irregular boundaries, where other analytic or numerical solutions are either unrealistic or impractical. This model is quite general in scope and should be applicable to a variety of similar particle transport and diffusion-type plasma problems.

The Monte Carlo code developed in this work has been applied to the determination of the electron energy distribution function and related parameters for a noble gas plasma created by α-particle irradiation. The radiation induced plasma involved was characterized by the following features:

1) a continuous internal volume-source of high energy electrons

2) an applied electric field (optional)

3) secondary electron production via ionization processes

4) losses via recombination and leakage across boundaries

The calculations were specifically carried out for a helium gas medium with an electron source rate from 10^{14} to 10^{22} (#/cm^3-sec), initial electron energies from 70 to 1000 eV, pressures from 10 to 760 torrs and E/P (electric field/pressure) ratios from 1 to 10 V/cm-torr.

For the lower source rates, it is observed that, in the zero electric-field case, the low-energy portion of the distribution function is quite close to a standard Maxwellian distribution. However, the high-energy portion (above the ionization potential) of the distributions is a rapidly decaying parabolic-shaped tail which can be crudely represented by a 1/(Energy) distribution. The addition of the electric field causes the distribution function in the low-energy region to shift towards Smit's (or Druyvesteyn's) distribution while the high-energy protion essentially retains its zero field shape. As the source rate increases beyond certain value (roughly 10^{18} cm^{-3}-sec^{-1} in the present case), the low-energy region begins to depart from the standard Maxwellian or Smit distributions and this departure can become quite large.

A major emphasis in this development was placed on computation efficiency. The present computation scheme with its variance and accelerated convergence techniques is thought to be quite efficient compared to alternate approaches.

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CHAPTER I

INTRODUCTION

A. Statement of the Problem and Objectives

Two major goals were set for this study. The first was to develop an efficient Monte Carlo simulation technique for solving radiation-induced plasma problems. This required adapting several variance reduction techniques in order to increase the Monte Carlo efficiency. The second goal was to apply the model developed herein to study the characteristics of a noble-gas plasma created by alpha-particle irradiation.

The major point of interest is the determination of the electron energy distribution in the nuclear radiation induced plasma. This distribution is of direct importance to current experimental studies at the University of Illinois where the possibility of directly pumping* gas lasers with nuclear radiation is under study (6). Recent results from these studies also show that nuclear radiation can be used to enhance the output from some type of electrically pumped lasers (5).

B. The Importance of Nuclear Radiation Produced Plasmas and the Physical Model

Nuclear radiation can be used in two ways: to directly pump the laser, or alternately, where an electric discharge

---

*"Pumping" of a laser is defined as the introduction of energy into the lasing medium required for population inversion. The electrical current which creates the discharge in the conventional gas laser is the pump in that case. Flash lamps are used for many solid state lasers.

serves as the main pump, to enhance the operation of lasers. The possibility of efficient coupling of lasers and nuclear reactors has generated an interest in the use of high-energy ion beams to pump lasers. To avoid radiation damage problems, gas lasers are generally thought of in this connection.

There are several important reasons for searching for more direct methods of coupling energy from reactor sources into lasers (8). One is the possibility that the resulting laser may offer unique characteristics, e.g., new frequencies and new methods of modulation and control. Simplified coupling could also offer weight reductions and improved reliability, which may be of advantage in space applications. Also, it may eventually become feasible to simultaneously extract several energy forms, e.g., laser and electrical power from a single nuclear station.

In most gas lasers the excited states, and consequently the inversion of population necessary for laser operation, are formed directly or indirectly by electronic collisions in a plasma generated by an electrical discharge. However, an alternate way to accomplish this goal is via nuclear radiation which can produce ionization and excitation through both direct interactions and interactions due to secondary-electron production. Given the high neutron fluxes available from nuclear reactors, the particles from neutron-induced nuclear reactions (e.g., α-particles from a Boron coating on the wall of a laser tube) can furnish the nuclear radiation

source. The description of the transport of both the primary radiation and the secondary electrons, from their point of birth throughout their path in the gas, is a key problem in the quantitative evaluation of the plasma. Therefore the development of nuclear-radiation pumping requires a thorough understanding of the radiation-induced plasma.

The following physical model is applied to the situation of a radiation-induced plasma. Pertinent quantities of interest include: electron energy distribution spectrum; average electron energy; and rate of energy loss.

The heavy-charged particles (α-particles) are born in coating and enter an adjacent gas. In the present calculations, the cylindrical geometry of the actual laser tube is approximated by a slab geometry (cf. Figure 1) with two parallel plane boron coatings separated by a gaseous medium. The α-particle radiation continuously creates high energy electrons throughout the gas volume (with energy E_o). The resulting plasma is a weakly ionized, three-component plasma (electrons, positive ions, and neutral gas atoms). It is assumed that the alpha-particle trajectory can be treated analytically using methods such as developed in (7). Further, this reference shows how to obtain the primary secondary-electron (δ-ray) energy spectrum. The difficult problem, however, is to follow the thermalization and further secondary production of these primary electrons.

Thus, the Monte Carlo simulation starts off by following these electrons on their life time histories, i.e., by simulating the course of their thermalization. Electrons go through various processes of collisions and scattering, resulting in a complex process of diffusion, energy degradation and secondary production, but finally,they recombine with positive ions or escape from the system,ending their histories.

With the radiation rates of interest here, the plasma is only weakly ionized and electrons mostly thermalize by collisions with the neutral background-gas atoms. In other words, collisions with ions and other free electrons can be neglected. In this sense, the problem is simplified in that it remains linear. However, some non-linearity enters in the following way. The recombination process depends on the ion density and spatial distribution. However, the ions are originally formed by ionizations which occur as the electrons slow down.

Another important characteristic is that the plasma is highly non-equilibrium. The thermalized electrons and ions form an approximately Maxwellian background, but superimposed on this is the high energy tail due to the electrons in the process of slowing. Also, the alpha particles themselves represent a non-equilibrium component.

In summary, the special features of the plasma system are:

1) Continuous internal volume source.

2) An applied electric field may or may not be present.

3) Finite cylindrical geometry--approximated here by slab geometry.

4) Electron-ion pair production and recombination processes.

5) The energy range of the electrons range from kilovolts to thermal (eV.).

6) The system represents a non-equilibrium plasma, but in a steady-state condition (or stationary).

7) Due to relatively small densities of electrons and ions compared with that of gas atoms, direct interactions between the electrons themselves or electron-ion collisions are neglected.

C. General Approaches and Methods of Solution

Possible approaches toward solutions of these types of problems (particle transport and diffusion) can be categorized as follows:

1) Analytical solution of the governing Boltzmann transport equation.

2) Numerical solution of the Boltzmann transport equation.

3) Direct analog simulation (Monte Carlo).

4) Mixtures of the above approaches.

The governing equation for this type of problem is the Boltzmann equation, and most classical methods have involved approximate analytic solutions of it. Solutions are possible only after various approximations and simplifications are made, and such solutions are often very restrictive and/or difficult to extend to actual situations of interest. More

or less the same drawbacks apply to numerical solutions. However, in this case approximations are necessary or the computation time becomes too long, especially as the dimensionality and the complexity of the problem increases. In fact, the computation time increases roughly exponentially with the dimensionality of the problem. Usually the governing partial differential and integral equations (coupled Boltzmann equations) are reduced to finite difference equations, and the requirements for stability and convergence severely limit the maximum step sizes of the independent variables. Further difficulties with the practical application of such approaches arise because it is often difficult to include realistic boundary conditions.

Direct simulation by the application of Monte Carlo techniques seems to be the better approach; sometimes the only approach for such problems. It by-passes the direct solution of the partial differential-integral equation, and generally no approximations and/or simplifications are necessary. Complicated boundary conditions can be handled easily, and the computation time increases at the most linearly with the dimensionality of the problem. However, computer time still may be a problem so that judicious selection of numerical schemes and variance reduction techniques are required.

Many methods have been devised in the past which involve a mixture of analytic, numerical, and Monte Carlo approaches.

In such situations, Monte Carlo is usually applied to the most difficult part of the problem. For instance, in the evaluation of the non-linear, five-dimensional collision integral in the Boltzmann equation, straight forward numerical quadrature would require months of computation time even on the present day fast computers. The Monte Carlo (statistical sampling techniques which closely resemble the actual collision phenomena) techniques can produce results within reasonable computation time (24). The Monte Carlo method may be defined as a numerical device (numerical experimentation) for studying an artificial stochastic model of a physical or mathematical process. This study may be approached by one of two methods. The first is the process of simulation (direct analog simulation) in which the particles - electrons and ions in the case of plasma systems, or photons in the case of radiative transfer - are represented by a game of chance in the computer. In the second method, which is non-simulation, the Monte Carlo technique is strictly used as a numerical stochastic device for the solution of a given integral or partial differential equations (24,25).

CHAPTER II

THE MATHEMATICAL MODEL: NUMERICAL SCHEME AND PHYSICAL PROBLEM

A. General Description of the Physics of the Problem

The plasma under study is a weakly-ionized three-component plasma, and is non-equilibrium as described in Chapter I. The α-particle radiation continuously creates high-energy electrons throughout the gas volume. The Monte Carlo simulation is to trace these electrons' life histories and their complex processes of diffusion and energy degradation. Since the diffusion process of the electrons through the medium is affected by the density of the positive ions and the other electrons present (background electrons), the resulting problem is non-linear.

1. Physical Processes Involved

The mechanisms by which particles interact with the atoms of the medium are elastic and inelastic collisions, by which the incident particle is slowed and dissipates some or all of its kinetic energy to the medium by the combined action of the above mentioned processes. The particle can also experience so called superelastic collision by which the particle collides with the excited atoms gaining some energy. Finally, the particle can collide and recombine with positive ions or can leak out of the system thus ending its life

history.

As described in Chapter I, the type of interaction which is involved in any particular collision is governed by the laws of chance. For large numbers of interactions, the frequency of occurrence of any given interaction is determined by the relative magnitudes of the interaction cross sections. Secondary knock-on electrons due to the ionization process may be capable of further interacting with the atoms and producing additional secondary electrons.

As the system reaches steady-state, a balance is reached such that the birth rate for new particles, i.e., the rate at which primary or source electrons enter the system plus the production rate of secondary electrons due to ionization should approximately equal the loss rate due to leakage and absorption or recombination.

Since the transport of radiation through a medium affects its absorption properties, the transport of individual particles is indirectly affected by the density of the other particles present, and this introduces some non-linearities into the system. We shall adopt a piecewise predict-correct technique to approximate the nonlinear system with a linear model.

We are concerned with the simulation, by random sampling of the scattering of the charged particles. The direct simulation of the physical scattering processes in such a way that the diffusion process is imitated by letting

the particles carry out a random walk, each step of which takes into account the combined effect of many collisions. The mechanisms by which electrons interact with the atoms of the medium are elastic, inelastic, and superelastic collisions as well as recombination with positive ions. The incident source electron is slowed and dissipates some or all of its energy to the medium by the combined action of the various scattering processes, until it escapes, or recombines with an ion (radiative energy losses are neglected). The probability that an interaction occurs is determined by the total collision cross-section. The type of interaction is then determined by the relative magnitudes of the individual cross-sections.

2. Relation to the Transport Equation

Although no direct use will be made of the governing Boltzmann transport equation in the sequel, we shall write it down briefly, in order to indicate the mathematical problems to be solved implicitly by the Monte Carlo method. It is a nonlinear integro-differential equation of the form

$$\frac{\partial f}{\partial t} + \bar{u} \cdot \nabla_r f - \frac{|e|}{m} (\bar{E} + \bar{u} \times \bar{B}) \cdot \nabla_u f = \left(\frac{\partial f}{\partial t}\right)_{\text{collisions}} \quad (1)$$

where f: number density distribution function

$\bar{B}$: magnetic field

$\bar{u}$: velocity of the particles

$\bar{E}$: electric field strength

t: time

r: spatial variable

In our situation $\overline{B}=0$ since the magnetic field does not exist. Further, if we assume an infinite medium and uniform source, $\nabla_r f=0$, the distribution function f depends only on energy. Then the above equation reduces to

$$\frac{\partial f}{\partial t} - \frac{|e|}{m}\overline{E} \cdot \nabla_u f = \left(\frac{\partial f}{\partial t}\right)_{\text{collisions}} \qquad (2)$$

The right hand side term is the collision term, which is the most difficult part of the equation. The effects of all relevant particle interactions must be included in this term. For the case of electron collisions with stationary gas atoms of uniform density, we can write the collision term as:

$$\left(\frac{\partial f}{\partial t}\right)_{\text{collision}} = \left(\frac{d N_{in} - d N_{out}}{dV \cdot dt}\right) \qquad (3)$$

where dN_{in} gives the number of phase space points (electrons) that are scattered into the phase-space volume dV by collision in time dt. Similarly, dN_{out} represents the number of points scattered out of dV by collisions in time dt. This Eq. 2 states that the change in the distribution function f are caused by collisions of various kinds and the external force due to the electric field.

The assumptions that enter into the derivation of the transport equation which carry over to the Monte Carlo

simulation include:

a) the scattering centers (background atoms and ions) are distributed at random, i.e., possible correlations between the positions of various atoms and ions are not taken into account.

b) In the absence of an electric field, the trajectory of the particle is idealized as a zig-zag path, consisting of flights interrupted by sudden collisions in which the energy and direction of the particle changed. The quantum-mechamical interference (electron diffration) resulting from the coherent scattering by several centers are neglected, and a particle, in the course of traversing the medium, interacts with one scattering center at a time.

The diffusion process in terms of the transport equation is analogous to the use of Eulerian coordinates in hydrodynamics, in that one asks about the flux at given points in space. By contrast, the Monte Carlo method uses Lagrangian coordinates; one attaches a label to a particular bit of fluid, i.e., a diffusing particle, and follows its history. Then, by sampling many histories, one is able, at least in principle, to solve any diffusion problem.

B. The Stochastic Model - Numerical Scheme

The essential approach to the nonlinear problem adopted here is the use of piecewise linearized steps. In each such step (an amount of time Δt along the time axis), the

dominate parameters, which characterize the nonlinear properties, are predicted and considered to be fixed with respect to the independent variables. During the time Δt, the system can be considered as more or less linear, so the conventional Monte Carlo simulation technique is used. The quantities pertaining to the given system are computed for each of a reasonably large number of independent particle histories. The desired parameter values are obtained by averaging the results over all of the histories. At the end of the step, the dominate parameters are corrected before beginning the next step. In each step (time interval Δt, or cycle), instead of computing the trajectory and angular deflection of an electron after each interaction, we perform a random walk calculation. Since each step of the random walk takes into account the combined effects of many individual interactions, we form a so-called condensed history by this approach. Let us describe the model in some detail, step by step.

1. The Geometry and the Coordinate System

The initial spatial geometry in this problem is a one-dimensional, finite slab (from z=0 to z=D) which is subdivided into uniform intervals called zones as shown in Figure 1. The energy range is from 0 to E_o (=1keV) which is also subdivided into three regions: $0 \sim 1$ (thermal energy region), 1 to ED2, and ED2 to E_0. Each of these

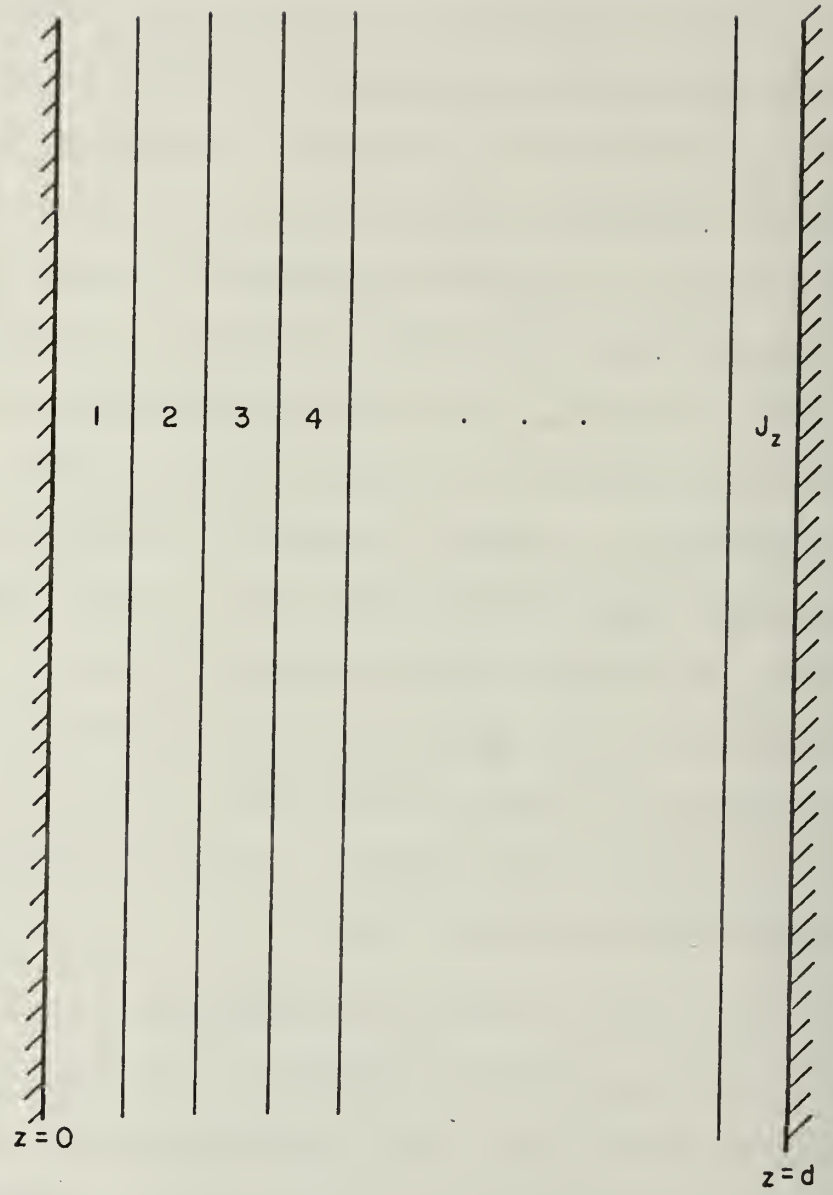


Figure 1. Slab geometry of the medium with subdivided zones.

regions is further divided into smaller uniform or logarithmic spacing (intervals). The particle number density distribution f(E,z) is a function of energy E and spatial position z and is generated such that particles with energy and spatial position falling into the same intervals are grouped together and normalized by the total particles processed. Although the system is stationary, we deliberately introduce the time variable for the convenience of recording output information and carrying out the calculation steps. The time serves as a clock, or we can imagine that the system begins in a transient state. Then, as time goes on it will eventually reach steady state. The storage of the timing information for individual particles is not necessary. Instead of following a single particle from the beginning to the end of its history, we follow a large number of particles, say N (which represent the sample particles of the whole system population) through a small time interval Δt (called the cycle time). Within this time interval, the system is considered to be linear, and the particles are processed more or less independently as in a conventional linear Monte Carlo model. At the end of Δt, called census time, we record data information for each particle (record particle state information). During this time interval (or present time cycle) some particles may experience collisions of some kind, some may not, and new particles (source particles, secondary particles produced

by ionization) enter the system. Some particles may be absorbed or escape from the system; their histories are therefore ended. This represents a random walk calculation, and each step of the random walk takes into account the combined effect of many individual interactions. The trajectory of a particle which is computed by this approach is called a condensed history. The residue particles (ionization produced secondary particles) are also set into motion, and their histories are followed separately. They are like all the other source particles in all respects. The complete description of particle histories is approximated by the condensed histories, or we take sequences of snapshots of all the particles in the system at various times to provide a moving picture of the history that can be used to estimate the quantities of interest. The path lengths travelled by the particles are also used as a clock to measure time, or equivalently, the variable t may be replaced by $S(t) = \int_{t_o}^{t} v(x)dx$. The trajectories of the particles (the condensed histories) are described by the arrays as indicated in Figured 2. The superscript denotes the cycle time number; the subscript denotes particle number where the index 0 refers to the initial state of the particle. Other notation includes E: the particle energy, z: spatial position, and U: the direction, and wt: the weight. When the particle has traveled a path-length DCEN (in the same duration Δt), a condensed history

i \ t	t_o	t_1	...	t_j	...	t_m
1	E_1^0	E_1^1	...	E_1^j	...	E_1^m
	Z_1^0	Z_1^1		Z_1^j		Z_1^m
	U_1^0	U_1^1		U_1^j		U_1^m
	wt_1^0	wt_1^1		wt_1^j		wt_1^m
2	E_2^0	E_2^1	...	E_2^j	...	E_2^m
	Z_2^0	Z_2^1		Z_2^j		Z_2^m
	U_2^0	U_2^1		U_2^j		U_2^m
	wt_2^0	wt_2^1		wt_2^j		wt_2^m
.	.	.		.		.
.	.	.		.		.
.	.	.		.		.
N	E_n^0	E_n^1		E_n^j		E_n^m
	Z_n^0	Z_n^1		Z_n^j		Z_n^m
	U_n^0	U_n^1		U_n^j		U_n^m
	wt_n^0	wt_n^1		wt_n^j		wt_n^m

Figure 2. Snapshops of the particles' condensed histories.

is sampled. Letting the particle carry out a random walk in each step (from state M to state M+1) takes into account the combined effect of many collisions. The sizes of the steps of the random walk, i.e., the pathlength intervals DCEN (equivalent to Δt) are chosen such that the total number of steps should be kept as small as possible. Too large a step size (Δt) may cause inaccuracies in the approximation. However, the length of the Monte Carlo calculation is directly proportional to the total number of steps. Thus, a compromise must be reached such that we choose as big a step size as possible without introducing intolerable inaccuracies. A reasonable initial value is chosen such that the particle with the average energy of the time cycle travels one mean free path, i.e., $\Delta t = D_{avg}/V_{avg}$. Different time cycles have different E_{avg} (V_{avg}) and D_{avg} so Δt may vary, but as steady-state is approached, Δt will not change much. By this technique we not only randomize and average the different particle samples, ensemblewise, but we also do the same (on the particle ensemble sets) along the time axis (averaging independent but equivalent time cycles). Trial and error results indicate that the optimum values of Δt (or DCEN) lie between 0.5 (D_{avg}/V_{avg}) 2.0 (D_{avg}/V_{avg}).

The maximum number of particles (N) that can be processed in each cycle is limited by the amount of storage available in the computer system. For the IBM 360/75 system

at the Illinois Computer Center, the storage of the data for 5,000 particles is easily accomplished. By playing Russian roulette, splitting, or similar techniques, the total number of artificial particles (N) can be increased by an order of magnitude. The end of one time cycle t_i is the start of the next time cycle t_{i+1}. While keeping track of the particles in a current time cycle at one time, we simultaneously record the data information after each particle reaches the census and extract the output parameter values after all the particles have been processed. In this way the storage requirements are reduced to a minimum level possible.

The limitation on N by the storage requirement may be further relaxed by the following technique. Instead of recording and tallying the output information and clearing or reinitializing all parameter values at the end of every cycle, we record the accumulated information for K continuous, and similar but statistically independent time cycles, then renormalize and reinitialize. In this way the total number of particles processed is KN, and if processing of a large number of particles is desired, we can use a larger value of K(K>1) at the expense of more processing time. The reason for this is based on the fact that the system being simulated is time independent. We have introduced the time variable artificially so that ergodicity holds, namely ensemble averaging is the same as time averaging.

2. Tracing Procedure

The simulation is initialized by introducing N particles with energy E_{in} [sampled from an initial guess for the number density distribution vs. energy], with spatial position z_i^0 (uniformally distributed throughout the spatial region), with direction u_i^0 ($u=\cos\theta$; θ: angle of flight with z axis) which is uniformly distributed between -1 and +1 and with weight wt_i^0. Volume particles are emitted uniformly throughout the medium and isotropically in direction; namely, at $t=t_o$:

$$E_i^0 = E_{in} \tag{4a}$$

$$Z_i^0 = r_i \cdot D \tag{4b}$$

$$u_i^0 = 2r_i - 1 \tag{4c}$$

where r_i: random number, uniformly distributed between 0, 1, or $r_i \in (0, 1)$

d: slab width or cylinder diameter

wt_i, E_{in}: weight and particle energy determined from initial distribution.

Once the particle data are determined, the geometry routine is entered. This includes the determination of the distance to boundary d_B, the distance to collision d_{col}, and the distance to census time d_{cen} (clock distance equivalent to Δt). These distances are defined by:

$$d_B = [(j+1)\Delta Z - Z]/u \quad \text{if } u > 0 \tag{5}$$

$$= (Z - j\Delta Z)/|u| \quad \text{if } u < 0$$

$$= \text{DLB (a large number DLB} \gg \Delta Z) \text{ if } u \approx 0$$

$$d_{col} = \lambda(E) \left|\ln r\right| = \left|\ln r\right| / \Sigma_t(E) \tag{6}$$

$$d_{cen} = D_{avg} \cdot DI = V_{avg} \cdot \Delta t \cdot DI \tag{7}$$

where r: random number uniformly distributed

j: zone number

Δz: spatial interval size

Σ_t: the total cross-section evaluated at the particles' energy

D_{avg}: the average value of D_{col} of N particles of the previous cycle. It is approximately one mean free path corresponding to E_{avg}: the average energy of the cycle.

DI: input parameter for controlling the cycle time interval.

The next step depends on which of these distances is the smallest.

a. <u>The System Without Electric Field (E_f=0)</u>

i) If the smallest distance is d_{cen}: the particle is advanced in position and time to census time.

$$z' = z + u.d_{cen} \tag{8a}$$

$$u' = u \tag{8b}$$

$$E' = E \tag{8c}$$

The particle data is stored, the energy is tallied, and

the density counter is incremented. Then we go on to process the next particle.

ii) If the smallest distance is d_B, the particle is advanced to the boundary such that:

$$z' = z + (d_B + 0.001 \cdot \Delta z) \cdot u \tag{9a}$$

$$j = \text{INT}\,(z'/\Delta z) + 1 \tag{9b}$$

$$d'_{col} = d_{col} - d_B \tag{9c}$$

$$d'_{cen} = d_{cen} - d_B \tag{9d}$$

where j is the zone number. If $j>JZ$ or $j<1$, then the particle is considered lost or has escaped from the system, and its history is ended. Otherwise the calculation and selection is repeated until the particle reaches the census time.

iii) If d_{col} is the smallest, the particle is first advanced to collision point and

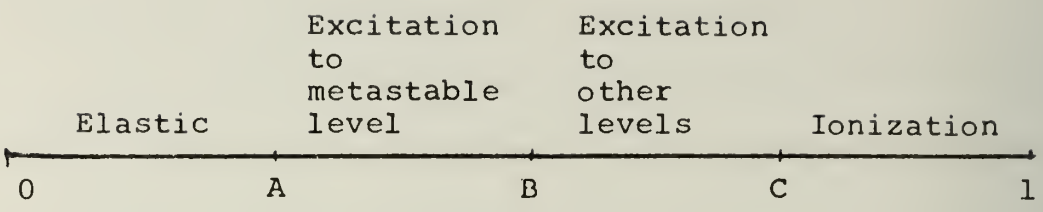
$$z' = z + u \cdot d_{col}$$

$$d'_{cen} = d_{cen} - d_{col} \tag{10}$$

Then the type of collision is specified. For specifying the collisional processes, we divide the whole energy range into two regions. Region I: energy range 0 to ED1 eV. Region II; energy range ED1 eV to E_o eV. Ed1 and E_o are specified by input parameters and are referred to as the energy dividing line and source particle energy, respectively.

If the particle's energy is in the range of Region I, three kinds of collisions are possible: elastic collisions, electron-ion recombination, and superelastic collisions (where electrons hitting an excited atom pick-up the excitation energy). If the particle's energy falls in Region II, it can experience four kinds of collisions; namely, elastic collisions and three types of inelastic collisions--excitation to metastable level, excitation to other levels, and ionization. For ionization, the secondary electron so produced shares energy with the primary electron, and the energy of primary electron before collision less the ionization potential is shared between the two electrons. The partition of the shared energy could be determined according to Goodrich's experimental distribution curve (31). But based upon Thomas' (1) calculation experience, the way in which the energy is partitioned does not have a strong influence on any of the calculated mean properties. Thus, for computational simplicity, as Thomas did in all his calculations, we choose the partition ratio 9:1. The secondary electrons produced via ionization are considered as new particles introduced into the system. Thus they are followed from their point of birth just like other particles. This is equivalent to the generation method for processing branched trees of samples.

The type of collision is determined according to Figure 3 using a random number (uniformly distributed



$$A = P_{el}$$

$$B = P_{el} + P_{met}$$

$$C = P_{el} + P_{met} + P_{exc}$$

$$P_{el} + P_{met} + P_{exc} + P_{ion} = 1$$

Figure 3. The probability model for determining the types of collision.

between 0 and 1) to play the law of chances.

b. With Electric Field Present

The coordinate axis z is defined as antiparallel to the electric field E_f. In the presence of electric field E_f, the state of motion of an electron is specified by its speed V and the direction cosine cos θ, where θ is the angle made by the line of flight with the z-axis at the time t. If an electron is in a state [E(V), u(cosθ), z, t], it will assume (after a flight along the orbit by Δt) the new state [E'(V'), u'(cosθ'), z+Δz, t+Δt]. These parameters are connected by the following relations:

$$V' \cdot \sin\theta' = V \cdot \sin\theta \tag{11}$$

$$mV'\cos\theta' = mV\cos\theta + eE_f \cdot \Delta t \tag{12}$$

$$1/2\ mV'^2 = 1/2\ mV^2 + eE_f \cdot \Delta z \tag{13}$$

$$E' = E + eE_f \cdot \Delta z \tag{14}$$

where m and -e are the mass and the electric charge of the electron, respectively. Here Δz is the projection of the path length L on the z axis. It can be obtained as follows;

$$\Delta z = \int_0^{\Delta z} V_z dt = \int_0^{\Delta t} (V \cdot u + \frac{E_f}{m} \Delta t)\ dt$$

$$= V \cdot u \cdot \Delta t + 1/2 \cdot \frac{E_f}{m} \cdot \Delta t^2 \tag{15}$$

In carrying out the geometry routine, it is suitable to use time directly as the clock. The determination of the distance to collision d_{col} (DCOL) and the distance to census

d_{cen}(DCEN) is accomplished as follows:

$$DCOL = \lambda \cdot |\ln r| \tag{16}$$

$$= 2/(1/\lambda_{(E)} + 1/\lambda_{(E')}) \tag{17}$$

$$DCEN = \sqrt{V_y^2 + V_z^2} \cdot \Delta t \tag{18}$$

$$V_y = V \cdot \sin\theta \tag{19}$$

$$V_z = V \cdot \cos\theta + \frac{E_f}{2m} \Delta t \tag{20}$$

where E: the initial energy of the particle

E': the energy of the particle after flight time Δt.

The next step is to determine which of the distances is smaller. If DCEN<DCOL, then the particle is advanced to the new state

$$E' = E + E_f \cdot \Delta z$$

$$z' = z + \Delta z$$

$$u' = \sqrt{E/E'} \cdot u + eE_f \cdot \Delta t \tag{21}$$

If $E' \leq 0$ or $z' > D$, $z' < 0$ then the particle is considered to have escaped from the system. If DCEN $\geq$ DCOL, the particle is advanced to collision point.

$$\Lambda t' = \Lambda t - DCOL \cdot \Delta t/DCEN$$

$$DCEN = DCEN - DCOL$$

$$z' = z + \Delta z \cdot DCOL/DCEN$$

$$E' = E + \Delta z \cdot E_f \cdot DCOL/DCEN \tag{22}$$

then the specific collision type must be determined.

c. Types of Collisions and Cross Sections

For the elastic collisions, the particle scatters off with angle of deflection θ and energy loss ΔE, the following formula is used (36).

$$\Delta E = \frac{2m}{M} (E-E_n) (1-\cos\theta_s) \qquad (23)$$

where θ_s: scattering angle (angle of deflection)

E: particle energy

E_n: target gas atom energy

m: electron mass

M: gas atom mass

E_n is selected according to a Maxwellian distribution, and the ΔE so formed may have either positive or negative values, indicating the loss or gain of energy respectively. For calculational simplicity, instead of selecting the deflection from the elaborate distributions, we use $\pi/4$ or $\pi/2$ deflection approximations, namely $\theta_s = \pi/4$ or $\pi/2$, then $\cos\theta_s = 0$ or 0.70711. Another reasonable alternative is to assume that the direction after collision is equally probably in all directions (isotropic scattering). We select this direction at random with uniform distribution, and based on Eq. 23 calculate $\cos\theta_s$ and ΔE, respectively, where

$$\cos\theta = 2r_i - 1 \qquad (24)$$

$$\theta_s = \theta - \theta_i$$

where θ_i: incident angle

θ: outgoing angle after collision

For the three kinds of inelastic collision cross sections we use approximate formula based on experimental data as correlated by Itoh and Musha (2). The formulas are expressed in the form:

$$\sum(E) = \frac{B(E-E_i)}{A+(E-E_i)^2} + C \qquad (25)$$

where the constants A, B, C, and E_i depend on the kind of collision and scattering angle. For the elastic cross section in helium, we use a single approximate formula for whole effective energy range based on Heylen and Lewis's paper (10), namely:

$$\sum_{el}(E) = 26\exp(-0.04E) \ (cm^{-1}) \qquad (26)$$

For the recombination cross section for helium (35), we assume the simple form:

$$\sum_{RCB}(E) = \mu(E)\cdot N^+$$
$$\mu(E) = 10^{-9}/V(E) \qquad (27)$$

where N^+: ion density

V: electron velocity

the superelastic cross section is

$$\sum_{Sel}(E) = \frac{0.109(19.8-E)}{0.25 + (E-19.8)^2} \cdot \frac{N^+}{3\cdot D_n} \qquad (28)$$

where N^+: positive ion density

D_n: gas atom density

E: electron's energy

3. The Prediction and Correction of Dominant System Parameters

There exists a single parameter, the ion density distribution $N^+(E,z)$, which completely characterizes the nonlinearity of the system. This simplifies the problem and suggests the following predict-and-correct scheme. We assume that the average mean free path (or Δt) and the ion density distribution $N^+(E,z)$ in the present time cycle also applies to the next time cycle, In other words, in each time cycle we use the predicted values of Δt and $N^+(E,z)$ from previous time cycle. At the end of present time cycle, we use the up to date information to renormalize and correct the value to be used for the next time cycle. As steady state is reached, the predicted and corrected values of the parameters converge. From the continuity equation

$$\nabla \cdot J = S - L \tag{29}$$

where J: the particle current flow in or out of the system

S: the source

L: the sum of losses

To start with, we assume that $\nabla \cdot J = 0$, so that

$$S = L = \alpha(E)\, N^+(E,z)\, N^-(E,z) \tag{30}$$

Here $N^-(E,z)$ is the electron number density, the key quantity we are calculating. To initialize the run we have to predict $N^+(E,z)$. It is reasonable to initially assume this distribution is uniform in z, and a maxwellian distribution in E, i.e., $N^+(E,z) = N_0 M(E)$. We also assume that $N^-(E,z)$ is the same as $N^+(E,z)$. Then we obtain

$$\begin{aligned} S = L &= \alpha(E)\, N^+(E,z)\, N^-(E,z) \\ &= \alpha(E)\, [N^+(E,z)]^2 \end{aligned} \tag{31}$$

$$\text{or} \quad S_0\, \delta(E-E_0) = \alpha(E)\, N_0^2\, M^2(E)$$

Integration of both sides gives

$$S_0 = N_0^2 \int_0^{E_0} \alpha(E)\, M^2(E)\, dE$$

$$\therefore\ N_0 = \left[S_0 \Big/ \int_0^{E_0} \alpha(E)\, M^2(E)\, dE\right]^{1/2} \tag{32}$$

This gives a starting value for the calculations. In later cycles the renormalization process involves integration of Eq. 29, with $\nabla \cdot J \neq 0$, i.e.,

$$\iint \frac{dJ(E,z)}{dz}\, dzdE = \iint S(E,z)dzdE$$

$$- \iint \alpha(E)\ \ N^+(E,z)\, N^-(E,z)dzdE - J_{esc} + J_s$$

which reduces to

$$J(Z=d) - J(z=0) = S_0\, d - \iint \alpha(E)\, N^+(E,z)\, N^-(E,z)dzdE$$

$$- J_{esc} + J_s$$

$$N_i^2 = \frac{S_0 d + J_s - [J(z=d) - J(z=0)] - J_{esc}}{\iint \alpha(E)\, M(E)\, \bar{n}(E,z)\, dz dE} \qquad (33)$$

where i refers to ith time cycle

J_{esc}: current due to escaped electrons

J_s: current due to secondary electrons produced by ionizations

$M(E)$: Maxwellian distribution (normalized)

$\bar{n}(E)$: electron number density distribution (normalized)

S_0: source rate

N_i: ion density distribution (normalized)

The value of N_i replaces N_0 in equation (33) at later time cycles. The value of N_i (N^+) enters the formula for the recombination cross section and superelastic cross section, thus it directly affects the rates of recombination and superelastic collision. Indirectly, it affects the balance of the system, or equivalently the rate of convergence of the Monte Carlo calculation. An adaptive correction procedure is used here. It is based on the value of the "balance factor" BF, defined as the ratio of the particles introduced into the system by source and ionization processes to the particles removed from the system due to recombination and leakage. We adopt a over-relaxation type of correction technique, the over-correction is used to speed up the over-all convergence rate. As defined before, if BF > 1, the system has more particles introduced

into than eliminated, but if BF < 1, the opposite is true. The over-correction factor is proportional to $(BF)^k$, i.e., to the kth power of the balance factor. The value of k initially chosen was k=2, but an optimum value can be obtained by trial and error.

CHAPTER III

VARIANCE REDUCTION TECHNIQUES

A. General Background

The Monte Carlo method (or method of statistical trials) consists of solving various problems of computational mathematics by the construction of some random process for each such problem, with the parameters of the process set equal to the required quantities of the problem. These quantities are then approximated by observations of the random process and the computation of its statistical characteristics, which are approximately equal to required parameters [from Schreider (15)]. Every Monte Carlo computation that leads to quantitative results may be regarded as estimating the value of a multiple integral. Suppose we have M random numbers in the computation system. The results will be a vector valued function $R(\xi_1, \xi_2, \ldots \xi_M)$ involving the sequence of random numbers $\xi_1, \xi_2, \ldots \xi_M$. This is an unbiased estimator of $\int_0^1 \ldots \int_0^1 R(x_1, x_2, \ldots x_M)$ $dx_1 \ldots dx_M$. For the sake of simplicity, we take the one-dimensional integral as a standard example. Let

$$\theta = \int_0^1 f(x)dx \tag{34}$$

where $f \in L^2(0,1)$ or $\int_0^1 [f(x)]^2 dx$ exists.

Define the relative efficiency of two Monte Carlo methods as follows. Let the methods call for n_1 and n_2 units of computing time, respectively, and let the resulting

estimates of θ have variances σ_1^2 and σ_2^2. Then the efficiency of method 2 relative to method 1 is defined as

$$\frac{n_1 \cdot \sigma_1^2}{n_2 \cdot \sigma_2^2} \tag{35}$$

Equation 35 is the product of two terms, the variance ratio σ_1^2/σ_2^2 and the labor ratio n_1/n_2. If $\eta_1, \eta_2, \cdots \eta_N$ are independent random numbers with uniform distribution between 0, 1 or $\eta_i \in (0,1)$; then the quantities $f_i=f(\eta_i)$ are the independent random variates with expectation θ. Therefore

$$\bar{f} = \frac{1}{N} \sum_{i=1}^{N} f_i \tag{36}$$

is an unbiased estimator of θ, and its variance is

$$\frac{1}{n} \int_0^1 (f(x)-\theta)^2 dx = \frac{\sigma^2}{n} \tag{37}$$

Accordingly the quantity $\bar{f}$, which has been determined by observation of the random process, is approximately equal to the required quantity θ (or in other words, it is an unbiased estimator of θ) with a probability which can be made as close as required to unity if a large number of trials is practical. We refer to the estimator $\bar{f}$ as the crude Monte Carlo estimator of θ (commonly referred to as Monte Carlo estimation).

Let us introduce another even less efficient method, namely hit or miss Monte Carlo. Suppose that $0 \leq f(x) \leq 1$

when $0 \leq x \leq 1$. We may draw the curve $y = f(x)$ in the unit square $0 \leq x, y \leq 1$, and θ is the proportion of the area of the square beneath the curve. Stating this formally, we write

$$f(x) = \int_0^1 g(x,y)dy \tag{38}$$

where $g(x,y) = 0$ if $f(x) < y$

$= 1$ if $f(x) \geq y$

Then

$$\theta = \int_0^1 \int_0^1 g(x,y)\, dxdy \tag{39}$$

The estimator

$$\bar{g} = \frac{1}{n} \sum_{i=1}^{n} g(\xi_{2i-1}, \xi_{2i}) = \frac{n^*}{n} \tag{40}$$

n^* is the number of occasions where $f(\xi_{2i-1}) \geq \xi_{2i}$
In other words, we take n trials at random in the unit square, and count the proportion of them which lie below the curve $y = f(x)$.

Historically, a hit or miss method was first propounded in the explanation of Monte Carlo techniques. It is the easiest to understand but one of the least efficient techniques. The rate of convergence and the variance (statistical error) is in general proportional to $1/\sqrt{N}$ where N is the number of samples. It is obviously impractical to gain a significant improvement of accuracy by merely increasing N. Therefore more efficient techniques for reducing the variance and/or increasing the efficiency

are very important. Monte Carlo experimentalists need wide experience and background in both the mathematics and the physics of the problem, and they have to exercise considerable ingenuity in distorting and modifying problems in the pursuit of variance reduction techniques. Statistical and inferential procedures are also important in order to extract the most reliable conclusions from the observational data.

The basic requirement of the Monte Carlo calculations is to establish how random numbers may be used to sample a function that describes, in a probabilistic fashion, a physical event. The procedure by which this is done follows from the fundamental principle of Monte Carlo (16), which may be stated as follows. If $p(x)dx$ is the probability of x lying between x and $x+dx$, with $a \leq x \leq b$

$$\int_a^b p(x)dx = 1 \tag{41}$$

Then $$r = P(x) = \int_a^x p(y)dy \tag{42}$$

determines x uniquely as a function of the random number r which is uniformly distributed on range (0, 1). The quantities $p(x)$, $P(x)$ are the probability density and the probability distribution functions, respectively.

With the development of large computers, the use of the Monte Carlo method in a wide range of problems has

increased rapidly. In particular, the method is applied to various physical problems such as plasmas (15), radiative transfer problems (21), neutron transport and nuclear reacter physics (29), etc.

The random walk type simulation can be briefly described in the following manner. One first introduces the basic physics of the problem into the computer in a probabilistic fashion. A system of coordinates and boundaries are defined and then, as a computer experiment, particles are released from the source. These particles are traced as they diffuse through a prescribed medium following the probabilistic interaction laws. The particles are followed until they escape from the medium or are absorbed or are converted to the thermal field.

The parameters pertinent to the evaluation of the desired quantities are recorded. One continues processing additional particles until adequate statistical estimates of the quantities of interest have been obtained.

When doing a Monte Carlo problem one focusses attention on three main topics. They are:

1. The development of the analogy for the probability processes (simulation).
2. The generation of sample values of the random variables on a given computing machine.
3. The design and use of variance reduction techniques.

The variance reduction methods are often strongly dependent on the probabilistic model, thus the greatest gains are often made by exploiting specific details of the problem, rather than by routine application of general principles.

B. Importance Sampling

The general idea of importance sampling is to draw samples from a distribution other than the one suggested by the problem. Then an appropriate weighting factor is introduced to correct the biasing caused by changing the original distribution. If done correctly the final results are essentially unbiased. The object is to concentrate the distribution of sample points in the parts of the region that are most "important" instead of spreading them out evenly. Thus, the probability of sampling from an interesting region is increased; the probability of sampling from unimportant or less interesting region is correspondingly decreased. Stating this formally, we have

$$\theta = \int_0^1 f(x)dx = \int_0^1 \frac{f(x)}{g(x)}\, g(x)dx = \int_0^1 \frac{f(x)}{g(x)}\, dG(x) \qquad (43)$$

for any functions g and G satisfying

$$G(x) = \int_0^x g(y)dy \qquad (44)$$

where g must be a positive valued function such that

$$G(1) = \int_0^1 g(y)dy \tag{45}$$

if γ is a random number sampled from the distribution G, then $f(\gamma)/g(\gamma)$ has the expectation θ and variance

$$\sigma^2_{f/g} = \int_0^1 \left(\frac{f(x)}{g(x)} - \theta\right)^2 dG(x) \tag{46}$$

We notice that if $g(x) = cf(x)$, or if g is proportional to f and if $c = \frac{1}{\theta}$ then $\sigma^2_{f/g} = 0$. This perfect situation does not exist, since we do not know θ. We always obtain an unbiased estimate for positive function g. Our object is to select g to reduce the standard error of our estimate.

Because the estimate is the average of observed values of f/g, we choose g such that f/g is as constant as possible in order to achieve a small sampling variance. While we intend g to mimic f, we generally restrict our choice of g to functions simple enough to allow analytic integration.

For the present plasma problem, the importance sampling technique is developed as follows: during the particle's (electron's) random walk, it suffers a large number of collisions with gas atoms, and these collisions may be elastic or inelastic or of other kinds. The probabilities of their occurrence depend on their cross section Σ_i. We have

$$\Sigma_t = \Sigma_1 + \Sigma_2 + \ldots \Sigma_M \tag{47}$$

where Σ_i: the cross section for ith process

Σ_t: total cross section or the summations of the cross sections of all the possible processes that the particle may experience.

Dividing both sides of equation 47 by Σ_t, we obtain:

$$1 = p_1 + p_2 + \cdots p_M \tag{48}$$

where $P_i = \Sigma_i / \Sigma_t$ the probability of ith process occurring as the particle experiences a collision. If we introduce weights w_i into equation 47 we obtain

$$\Sigma_t' = w_1 \cdot \Sigma_1 + w_2 \cdot \Sigma_2 + \cdots w_M \cdot \Sigma_M \tag{49}$$

Similarly we have

$$1 = p_1' + p_2' + \cdots p_M' \tag{50}$$

After the application of the weights, we put more weights on the interesting or more important events. Then their artificial probabilities are greater, therefore we can get better estimates of the important parameters. Coincidently, such a linear weighting scheme can only be applied to the elastic collision process in our system. The other collision processes involve appreciable changes in the particle's energy (catastrophic collision). Also cross sections are energy dependent, these nonlinear effects prevent the application of above mentioned weighting scheme to inelastic collision processes. By looking at the cross section values, in the low energy region, the elastic cross section is by

far the largest by order of magnitude. Others have shown that the elastic process does not strongly influence the estimated parameters that we are interested in (1, 2). As an electron makes an elastic collision, it loses only a small amount of energy while making a small angle deflection. In fact, most other workers simply neglect elastic loses if an electric field is present (1, 2, 10). In our case, with E_f=0, elastic effects must be included. In the low energy region ($\approx$ 0 eV to 20 eV), the energy of a majority of the particles lies below 1 eV and over 90% collisions are elastic collisions, and only a few collisions are inelastic.

The collision process subroutines are a time-consuming part of the simulation calculations. If we can supress the elastic processes by a factor of k_{el} the chances of all other processes are increased by approximately the same factor. Therefore we convert more computing time to processes which contribute more strongly to the quantities of interest. The following formulation provides the theoretical support for this. In lieu of equations 47-50, the p_i are the original probabilities (undistorted probabilities) while the p_i' are the weighted probabilities. Then the correction factors are introduced as follows; at energy E, we have

$$C_1 = p_1/p_1', \; C_2 = p_2/p_2' \; . \; . \; . \; C_M = p_M/p_M' \qquad (51)$$

$$\text{or} \quad C_i = p_i/p_i' = \frac{\Sigma_i \cdot \Sigma_t'}{\Sigma_t \cdot \Sigma_i w_i} = \frac{\Sigma_t'}{\Sigma_t} \frac{1}{w_i} \tag{51a}$$

If we let $w_1 = \frac{1}{k_{el}}$, $w_2 = w_3 = \ldots w_M = 1$

then from (51) we have

$$C_1 = \frac{\Sigma_1 \cdot \Sigma_t'}{\Sigma_t \Sigma_1 \cdot w_1} = \frac{\Sigma_t'}{\Sigma_t} \frac{1}{w_1}, \quad C_i = \frac{\Sigma_t'}{\Sigma_t} = 1, \quad i \neq 1 \tag{52}$$

let $\Sigma_1 = \Sigma_{el}$ namely we introduce weight on elastic cross section only. Since $\Sigma_{el}(E) >> \Sigma_i(E)$, $i > 1$, $\forall_i$ then

$$\frac{\Sigma_t'(E)}{\Sigma_t(E)} \simeq \frac{\Sigma_{el}'(E)}{\Sigma_{el}(E)} \qquad w_1 = \frac{1}{k_{el}} \tag{53}$$

and $$C_1 \simeq w_1 \frac{1}{w_1} = 1, \; C_i \simeq \frac{1}{k_{el}} \quad (i \neq 1) \tag{53a}$$

Equation 53 holds for low energy region, which is approximately independent of energy.

C. Russian Roulette and Splitting

In general, the sampling is done such that we examine the sample and classify it as being in some sense "interesting" or "uninteresting". We are willing to spend more than average amount of work on the interesting samples and on the contrary, we want to spend less effort on the uninteresting ones. This can be done by splitting the interesting samples into independent branches, thus resulting in more of them, and by killing off some of the uninteresting ones. The first process is splitting and the second Russian Roulette.

The "killing off" is done by a supplementary game of chance. If this game is lost, the sample is killed; if it is won, the sample is counted with an extra weight to make up for the fact that some other samples have been "killed". The game has a certain similarity to the Russian game of chance played with revolvers - whence the name.

For the present plasma system we divide the whole energy spectrum into two regions, the low energy region I (0 eV to ED1 eV) and the high energy region II (ED1 to E_0). Here E_0 is energy of source particles, which is the highest energy the particle can have. ED1 is the energy region dividing line, which can be chosen as any value between 5 eV and 100 eV depending on the initial guessed energy distribution. In region I, the number density is high, and the elastic process is the dominant process. As we mentioned earlier, the elastic process does not contribute much, so Region I is classified as uninteresting. Each particle in this region (particles with energy less than ED1) is assigned a weight k1($k1 \geq 1$). In other words, each particle plays the role of k1 particles.

In region II, classified as interesting region, each particle carries a weight w_2 ($w_2 = {}^1/k_2$, $w_2 \leq 1$). Namely, each particle in this region is split into k_2 particles with weight w_2.

As particles cross over to other regions, care must be taken to account for killing off and splitting effects.

For instance, a particle in region I may acquire enough energy, either from electric field or by superelastic collision with the excited atoms, to cross over to region II. Then we should generate k_3 particles ($k_3 = k_1 \cdot k_2$) in region II with the same energy.

Particles from the high-energy region may lose part of their energy by inelastic collision such that they cross over to the low-energy region. Then killing off should be effective. For every k_3 such particles that cross over from region II to region I, only one particle survives. The values of k_1 and k_2 can be chosen according to the total number of particles in the system to be processed, the source rate, and related accuracy requirements. They are input parameters.

D. Initial Guess

Monte Carlo methods comprise that branch of experimental mathematics which is concerned with experiments on random numbers. The user, like the experimental physicist needs theory and knowledge to give structure and purpose to his experiments, and as experimental work provides growing insight into the nature of a problem and suggest appropriate theory. Good Monte Carlo practice should keep this relationship as a general maxim.

The basic procedure of the Monte Carlo method is the manipulation of random numbers, but these numbers should not

be employed prodigally. Each random number is a potential source of added uncertainty in the final result. Thus it will usually pay to scrutinize each part of a Monte Carlo experiment to see whether that part can not be replaced by an exact theoretical analysis contributing no uncertainty. In other words, exact analysis should replace Monte Carlo sampling wherever possible. Sometimes reliable intuition would aid in increasing the efficiency of Monte Carlo calculations. For the plasma system we are simulating, the straight-forward approach would be to follow N source particles on their life time history, until they lose energy sufficient by collisions to reach a thermal equilibrium. Over 50 inelastic collisions generally occur, and the probability (inelastic cross sections) for inelastic processes is low. Consequently, the particles travel a relatively large distance which consumes a good amount of time. Thus a large number of time cycles would be required before the system reaches steady state. To avoid this, we use our intuition, to start off with a guessed initial distribution. The electron energy distribution f(E) (or electron number density distribution) is a function of the electron's energy E. Initial particle data is generated using this distribution, and this can save considerable irrelevant computations. This idea is simple, yet very useful and effective. Without an initial distribution, the problem would require hundreds of time cycles to

converge. However, with a reasonable guess, good results have been obtained in as little as tens of time cycles. Of course, the better the initial guess, the faster the convergence.

E. Antithetic Variates

When we estimate an unknown parameter θ by means of an estimator t, we may seek another estimator t' having the same (unknown) expectation θ as t but a strong negative correlation with t. Then $1/2(t + t')$ will be an unbiased estimator of θ, and its variance is

$$\mathrm{Var}[\tfrac{1}{2}(t+t')] = \tfrac{1}{4}\mathrm{var}(t) + \tfrac{1}{4}\mathrm{var}(t') + \tfrac{1}{2}\mathrm{cov}(t,t') \qquad (54)$$

where cov(t,t') is negative, and

$$\mathrm{var}(t) = \mathcal{E}\left[(t-u)^2\right]$$

$$\mathrm{cov}(t,t') = \mathcal{E}\left[(t-u)\cdot(t'-u')\right]$$

u,u' are the mean of t,t' respectively, and $\mathcal{E}(x)$ is the expectation of the random variable x.

It is possible to make var(t+t') smaller than var(t) by suitably selection t'. For example, 1-r is uniformly distributed whenever r is, and if f(r) is the unbiased estimator of θ, so is f(1-r). When f is a monotone function, f(r) and f(1-r) will be negatively correlated. Thus we could take

$$\tfrac{1}{2}(t+t') = \tfrac{1}{2}\, t(r) + \tfrac{1}{2}\, f(1-r) \qquad (55)$$

as an estimator of θ.

The name and idea of antithetic variates was first introduced by Hammersley and Morton (13, 14) during attempts to improve Buffon's needle experiment for estimating the value of π (3.1415926).

The main idea of antithetic variates is based on the underlining theorem [from Hammersley and Morton (12)] which can be stated informally as follows: "Whenever we have an estimator consisting of a sum of random variables, it is possible to arrange for a strict functional dependence between them, such that the estimator remains unbiased, while its variance comes arbitrarily close to the smallest that can be attained with these variables". As the name implies, antithetic variates are the set of estimators which mutually compensate each other's variations. Essentially, we rearrange the random variables by permuting finite subintervals in order to make the sum of the rearranged functions as nearly constant as possible. From the practical viewpoint, the mathematical conditions imposed by antithetic variates to the Monte Carlo calculation are quite loose and flexible. It is relatively easy to find a negatively correlated unbiased estimator to produce an efficient variance reduction scheme.

A system of antithetic variates is obtained by simple transformations based on a stratification of the interval (12). The transformations are constructed in such a way

that the efficiency of the method will increase as a higher power of M (the number of antithetic variates taken). The transformations considered are linear combinations of the values of the function f at a number of points. Thus a correlated stratified sampling technique is developed, and its efficiency generally exceeds that of crude sampling by a factor M^3.

The following useful transformations are obtained in this manner:

$$t_1 = \frac{1}{n}\sum_{i=1}^{n} \{\alpha f(\alpha r_i) + (1-\alpha)\, f[\alpha+(1-\alpha)r_i]\} \tag{56}$$

$$= \frac{1}{n}\sum_{i=1}^{n} G_\alpha f(r_i)$$

$$t_2 = \frac{1}{n}\sum_{i=1}^{n} \{\alpha f(\alpha r_i) + (1-\alpha)\, f[1-(1-\alpha)r_i]\} \tag{57}$$

$$= \frac{1}{n}\sum_{i-1}^{n} \mathcal{L}_\alpha f(r_i)$$

The value of α is between 0 and 1, the variance $\mathrm{var}(t_j)$ has a minimum at some value of α. An adequate rule of thumb is to choose α by finding the root of

$$f(\alpha) = (1-\alpha)\, f(1) + \alpha f(0) \tag{58}$$

Another useful transformation is

$$t_3 = \frac{1}{m}\sum_{j=0}^{m} f\left(\frac{r+j}{m}\right) = U_m f(r) \tag{59}$$

In general, the variance of crude Monte Carlo is $var(t) = 0(m^{-1})$ while the variance of t_3 is $var(t_3) = 0(m^{-2M})$, $(M > 1)$. The simplest form of antithetic transformations have proved quite successful in neutron transport calculations.

The general notion and a simple form of antithetic variates are applied in our present calculations. High efficiency gain can be obtained easily if it is used sparingly and at judicious points in the computation. We have used the random number $r_i (r_i \in (0,1))$ most of the time for playing the law of chances, and $1-r_i$ is another random number of the same kind which is the image of r_i. The two are used together in good many places where repeated use of r_i is required. This serves the purpose of two antithetic variates and cuts the labor in half (same random number r_i being used twice). Equations 55 and 59 have been used in the initial data preparation program and source routine where initial particles states (E_i, u_i, z_i, wt_i), E_i are generated according to input initial distribution. For instance:

$$
\begin{aligned}
&u_i = 2r_i - 1, \quad u_{i+1} = 2(1-r_i) - 1 \\
&z_i = r_i \cdot d, \quad z_{i+1} = (1-r_i) \cdot d \\
&E_i = E_k + r_i \cdot \Delta E_k, \quad E_{i+1} = E_k + (1-r_i) \cdot \Delta E_k \qquad (60) \\
&E_i = E_0 \text{ for source particles.}
\end{aligned}
$$

Here k is an energy index, or kth energy interval. Wherever r_i appears, r_i and $1-r_i$ are used interchangeably.

Thus we are generating source particles from diametrically opposite directions, or from symmetric locations.

F. Double History (Double Processing) Technique

In the particle tracing routine, using the general idea of antithetic variate technique, we have adopted a "so-called" double history processing technique which is described as follows;

a) In the course of tracing the particle's history, in each time cycle, we use the transformed random number $\lambda \cdot |\ln r|$ to decide the distance to collision $d_{col\ 1}$ and go on until the particle reaches census time. However, we process the same particle twice under the identical initial condition except that we use $\lambda \cdot |\ln(1-r)|$ as the distance to collision $d_{col\ 2}$. Both sets of history are ta lied but only one set of particle data is'stored. This way each particle is processed twice independently but correlated in such a way that they compensate each other's variation (variance).

b) Another alternative for double history processing is, to play a dual direction random walk instead of dual collision distances. We process the same particle twice in such a way it looks like there are two identical particles emerging into the system in two diametrically opposite directions. Again both histories are tallied, but only the original particle's data is stored.

The two versions of the double history processing technique increase the labor (computation time) by a factor of 1.2 to 1.5. The efficiency gain is difficult to specify. At least it is certain that the gain is more than double the total number of the particles in the system.

The purpose of dual processing is to compensate each particle's variation and minimize the variance (statistical errors). One set of particle data in dual processing is thrown away, while the other set is stored just like normal processing. Which one of the two resulting sets is saved is completely random.

CHAPTER IV

MONTE CARLO SIMULATION CODE

A. Introduction

This chapter presents the complete Monte Carlo simulation program, including an input, output, main flow chart, and the background theory and techniques incorporated. This program implements the condensed history approach that was described in Chapter II together with various variance reduction techniques described in Chapter III.

The basic Monte Carlo calculation can be described most easily by reference to the simplified flow chart shown in Figure 4. By means of this flow chart we shall follow the particle tracing process, making relatively brief comments on the various steps implied by each box, on each routine, and on the main program variables. The program is written in FORTRAN IV and is designed to be run on IBM 360/75 under the HASP-MVT system.

B. Calculational Procedure and Program Description

To obtain an overall view of the calculations, we note that there are three basic steps involved in the simulation process. The first is the initialization of all parameter values, i.e., prepare the particle data and predict the unknown dominate parameter values. The second is the main loop of particle tracing which generates census information. The third uses the census information and takes tallies to estimate the histograms (electron energy or number density

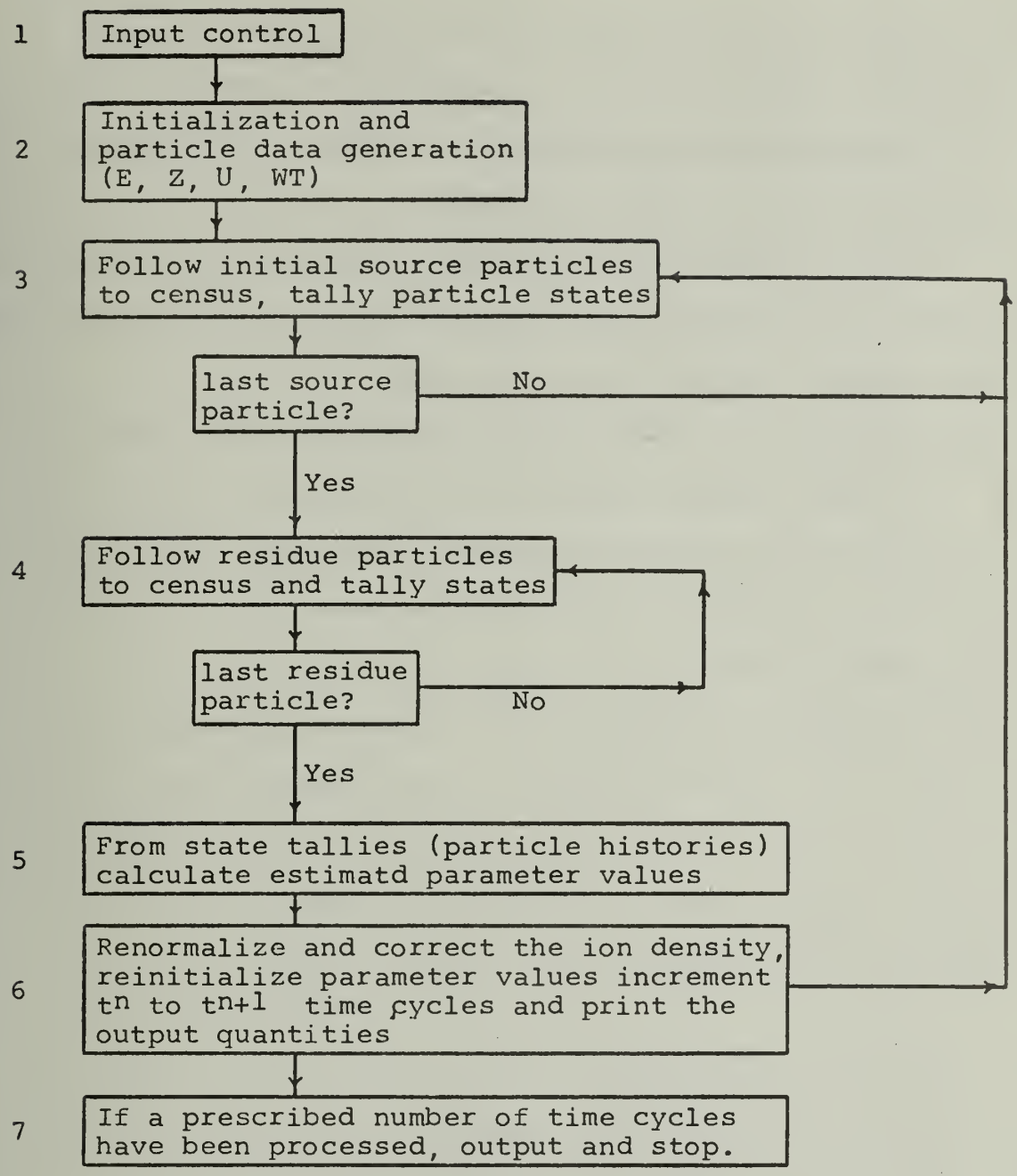

1
Input control
2
Initialization and particle data generation (E, Z, U, WT)
3
Follow initial source particles to census, tally particle states
last source particle?
No
Yes
4
Follow residue particles to census and tally states
last residue particle?
No
Yes
5
From state tallies (particle histories) calculate estimatd parameter values
6
Renormalize and correct the ion density, reinitialize parameter values increment t^n to t^{n+1} time cycles and print the output quantities
7
If a prescribed number of time cycles have been processed, output and stop.

Figure 4. Flow chart of the Monte Carlo simulation code.

frequency distribution vs. energy), and parameter values. Finally the dominate parameter va ues are corrected and the program returns to the first step.

Let us follow the logic flow diagram (Figure 4) in the order of the number marked on the left hand side of the boxes, and describe their individual functions.

1. Input Control: The main program is usually compiled and the loaded version is then stored on disk storage, ready for execution. In order to offer a wide flexibility, the following input parameters are used to control the program runs.

   a) NDISK: program start control. The program can start from the beginning (cycle 0), or it can start from the stopping point of the previous run. This feature enables long runs to be broken up into several short runs. It also offers debugging flexibility and economy of computer time. While a long run may run up to 150 time cycles, we can always break it up into multiple numbers of fives and tens cycles. Thus we can adjust other parameter values on a cut and try basis without wasting much computing time. The input parameter for this control purpose is NDISK: input 0 for storing from very beginning; input 1 for starting from the latest tenth cycle of last

run; input 2 for starting from the latest fifth cycle.

b) K1, K2, and ED1: Regional weights and dividing energy. The Russian Roulette and splitting variance reduction techniques use three input parameters to control the amount of killing off and/or splitting of particles. This also determines where to divide energy regions for the Russian Roulette and splitting, assuming that the option to use Roulette is selected. The input parameters are K1: the weight of particles in region I ($K1 \geq 1$), K2: the inverse of the weight w2 of particles in region II where $w2 = 1/K2$ ($K2 \geq 1$), ED1: the energy dividing line, namely (0 to ED1) is region I, (ED1 to E_0) region II where the energies are in electron volts.

c) NTC: The total number of time cycles to be run.

DTC: The input parameter to control the length of census time Δt of the time cycles. In terms of distance travelled by the particles, Δt is equal to a fraction or multiple of one mean free path , corresponding to average energy of particles in the system.

d) NTP: The total number of particles that actually exist in the simulation system.

NTW: The artificial* total number of particles in the system during Russian Roulette and splitting games.

NS: The number of source particles injected into the system during each time cycle.

e) KELC: The input parameter that controls the importance sampling option of the program, i.e., the multiplying factor used to suppress the elastic cross section (reduces the probability of elastic process by a factor KELC).

f) EDP: The input value of the ratio of the electric field strength to the pressure.

PDPO: The input value for the reduced pressure of the system ($^{p}/_{p_0}$ where p_0 = 1 torr).

g) NIP: The input parameter used to control double processing: NIP = 2 for double processing, NIP = 1 for single processing.

IUSN: IUSN = 1 for dual-collision type double processing

IUSN = -1 for dual-direction type double processing

---

*The total number modified by scaling and weighting factors.

h) D: The input value of the width of the slab (diameter of the cylinder) which defines the external boundaries of the medium.

JZ: The number of zones the slab is divided into, or the number of internal zones.

i) NCUM: Inp t control to give cumulative results (time average) over the time cycles or a cumulative average over NCUM time cycles.

NAVP: Input constant to control the power of Δt, (or ΔD) namely Δt_i**NAVP is the weight of the cycle to be used for cumulative results. These two parameters are used to implement antithetic variates techniques along the time axis.

j) EO: The energy of source particles.

SR: The rate of the source particles entering the system.

k) FID: An array that contains the initial guess distribution (number density vs. energy).

l) NUSC: An input parameter used to control the up-scattering elastic collision process; NUSC = 1: with upsacttering, NUSC = 0: without upscattering.

2. Data preparation: The initialization is entered only once during the calculation, where the time cycle is 0 (or at time t_0). After the input phase, all the pertinent

parameters are set to their proper permanent or temporary values. Before entering the next phase to trace the particle histories, several dominate parameter values must be predicted. The data preparation routine is called in to generate particle data (E_i: energy, u_i: direction of travel, Z_i: position, Wt_i: weight) based on the guess for the initial distribution (generate machine particles). Then the average energy of the system is calculated and is used to predict the census time (Δt or equivalently DCEN) as well as the number of ions(N^+).

3. Particle tracing: With the point of origin, direction of propagation, and energy (velocity) known for the initial source particles, the next phase follows the particles through a series of stochastic interactions until the census time is reached, and the particle data and parameters values are tallied and updated. During the course of tracing the particle histories, all the relevant events are recorded and later on can be interrogated to provide the output quantities of interest. This section of the program is the central part of the main program. It contains the main loop for tracing all the particles in the system in a self consistent way. Most of the variance reduction techniques are incorporated here, including double processing, Russian Roulette, and splitting, as well as the various versions of

importance sampling techniques.

4. Secondary particle tracing: The residue particles, i.e., particles generated by ionization collision process (the secondary electrons so produced) are treated in all respects like the regular source particles, except that their starting positions and time coordinates as well as directions are those associated with the particles that generated them. These residue particles may go further and produce other residue particles (secondary electrons) if their energy is high enough, thus forming a short production chain. The probability of such chain production is small however, since the average energy of the secondaries is quite low. The end of the main loop comes after all such residue particles are processed.
5. Data calculations: The details of the phase of the computations depend upon the specific goals and character of study. Our primary interest is the particle energy distribution (or number density vs. energy). This frequency distribution and other pertinent parameters are estimated (or calculated) using the stored data from various parameter counters in the main loop (tallied information) as well as tallied histories. The quantities of interest include local values (for the current time cycle only) and the cumulated values from several time cycles. After these calculations, the next phase is to prepare for the processing of new time

cycle.

6. Normalization and printout: Up to this stage, all the output quantities have been calculated. Next the output information is printed out, and at the same time, if the cycle number is the multiple of five, all the particle data and related parameter values are stored on the disk. Then the next run can be read off of the disk and the process can proceed from where we left off the last time. All the parameter values are again initialized, and new source particles are generated for the next time cycle. Particles that have escaped from the system or have been absorbed create holes in the particle data storage which are filled up by the new source particles and the residue particles produced during the time cycle. Before going on to the next cycle, the ion density is renormalized and corrected in a semiadaptive way according to a balance factor BF. The ion density distribution parameter N^+ is a dominate parameter since it affects several processes such as the rate of recombination and the rate of super-elastic collision (refer to Equations 27 and 28). It is corrected in such a way as to accelerate convergence, till the system reaches a balanced situation. Then increment time from t^n to t^{n+1}. The output quantities are the following:

   a) The kind of gas in the medium, source particle energy, pressure, slab thickness, and Δt the time interval of this cycle.

b) The number of time cycles, the time in seconds, the number of source particles generated during the cycle time, and the average energy of the particles in the system.

c) The number density distribution vs. energy, the single cycle distribution, the cumulated distribution, the number-density deviation, the average-energy deviation, the average energy, and the energy interval vs. energy.

d) The number density and the average energy vs. z (position zone).

e) The ion distribution (N_+), the number of ionizations (NIZN), the number of escaped particles (NES), the number of absorbed or recombined particles (NAS), the number of super-elastic collisions (NSE), the number of excitations to metastable levels (NMET), and the number of excitations to other levels (NEXC).

f) All the input control parameters as listed in section IV-1.

g) The electric field strength (EF), the source rate, the W-value, the average energy of escaped particles, and the average energy of absorbed particles.

h) The number check on the density disbributions.

All the above outputs include both current cycle values and the cumulated values over the past cycles.

7. Final checks: The last stage is to check whether the prescribed number of time cycles have been processed, adequate statistics have been collected, and all the useful data have been stored on the disk. If so, the program stops.

Further programming details are provided in Appendix

CHAPTER V

RESULTS

A. Convergence and Reliability

The present Monte Carlo Model is a predict-correct iterative scheme, with semiadaptive control ability. For such an iterative procedure, our main criteria for the evaluation and determination of convergence are based on the following inferences:

1. The balance factor (BF) as defined in Chapter II (Section II-B-3) signifies whether or not the system has reached steady state, i.e., converged to a final solution. At steady state, the value of BF should be approximately equal to unity. It may approach to unity in both directions, and due to semiadaptive control procedure used, it may oscillate around unity. Larger amplitude oscillations are observed at first, but they rapidly damp out.
2. The estimated values of the major parameters, e.g. the average energy and the W-value show a similar fluctuation, and then they converge to nearly constant values as steady state is approached.
3. The validity of the convergence has been checked using test problems where analytic results are available. A good comparison has been obtained, showing that the program and the model are working correctly, free of obscure errors.

B. Error Estimation and Analysis

1. Error Analysis

1. As mentioned in early chapters, Monte Carlo simulation is equivalent to performing mathematical experiments, the results being based on observations of such experiments. From this analogy we can derive the following procedures for the analysis of errors or accuracies of our calculations.

It is convenient to subdivide experimental errors into three broad types, namely: random errors, systematic errors, and blunders. In general, the experimental error is some additive function of all three, while blunders can hopefully be eliminated. We shall describe them in detail in following sections.

a. Random errors - such errors are of great concern in Monte Carlo type calculations. They generally involve statistical fluctuations or deviations, representing the difference between the singly measured value and the best value of a set of measurements, i.e., the difference between the arithmetic mean and the true mean. Sometimes such errors are referred to as elementary (or inherent) errors in the measurements. The commonly used measure of random errors is the variance or standard deviation.

b. Systematic error - a systematic error tends to have the same algebraic sign, i.e. it is either an additive or subtractive quantity introduced in the measurement

process. It is an unpleasant and insidious contribution which is not generally amenable to statistical treatment. Thus such errors seriously impair the reliability of the estimation. Typical examples include:

i) Incorrect assumptions or approximation in the representation of certain processes.

ii) Constructional faults and mistakes in the algorithms or subroutines.

iii) Inadequate regard of constancy of experimental conditions or inadequate sampling techniques (biased).

c. Blunders - these are outright mistakes which should be corrected by all means. Possible examples include:

i) Incorrect logic, misunderstanding of the problems.

ii) Errors in transcription of data.

iii) Mistakes in constants used.

iv) Confusion of units.

In any type of calculation, the systematic error as well as blunders should be removed. One way for detecting such errors is to compare the program against some known reliable solutions. Only the random errors are subject to reduction by the various treatments amenable to attack by variance reduction technqiues.

The precision in an estimated (mean) value is proportional to the reciprocal of the statistical error and is

high if the statistical error is small, i.e. the accuracy is high if the net systematic error is small. Usually, but not necessarily, high accuracy implies small statistical errors as well.

As discussed in later sections, our model and program has been checked against several test problems, and good agreement has been obtained. Therefore, it can be assumed that any serious systematic errors have been removed and that the program is free of blunders. Thus, we shall concentrate on the analysis of random errors.

No thorough analysis of variance has been made. Due to the intricate way that the histories calculated during a given time cycle depend on previous time cycles, a meaningful variance estimate beyond the first time cycle seems to be out of the question. However as the system reaches steady state, the deviations or variations (statistical fluctuations) of the estimated parameters can be estimated by means of standard deviation (or variance) over subsequent time cycles. Namely, we use the following formulation:

$$S_i = \left[\frac{\sum_{j=1}^{n} (f_{ij} - \bar{f}_i)^2}{n} \right]^{1/2} \quad \forall\, i \tag{61}$$

where s_i: the standard deviation at the ith energy interval over n consecutive time cycles.

f_{ij}: the parameter value (density distribution function of ith energy interval, at jth time cycle.

$\bar{f}_i$: the average parameter value of ith interval over n time cycles.

A heuristic approach was adopted to measure local deviations or statistical fluctuations at each time cycle. This provides a relative magnitude of deviation or dispersion which can be used to compare the various variance reduction techniques. The approach is described as follows:

The estimated major frequency distribution (the electron energy density distribution function in our case) is obtained in the form of histogram. The abscissa of the histogram is divided into so-called class intervals (energy intervals in our calculations). In each such interval an erect rectangle (block) of heigh f_i and width E_i is formed. This block-area type of distribution is the fitted frequency distribution curve. We devise a numerical description of local deviations by defining:

i) the location index of the center of the erected rectangles in the histogram as i and with abscissa value E_i.

ii) the spread or dispersion around the center.

The total number of particles in each class interval (energy interval) is proportional to the area of the rectangular flock ($f_i \Delta E_i$), the particle's energy in this class interval falls in the range ($E_i - \Delta E_{i/2}$, $E_i + \Delta E_{i/2}$) with overall average energy $\overline{E}_i = E_i$. Then the following relationship holds (refer to Figure 5):

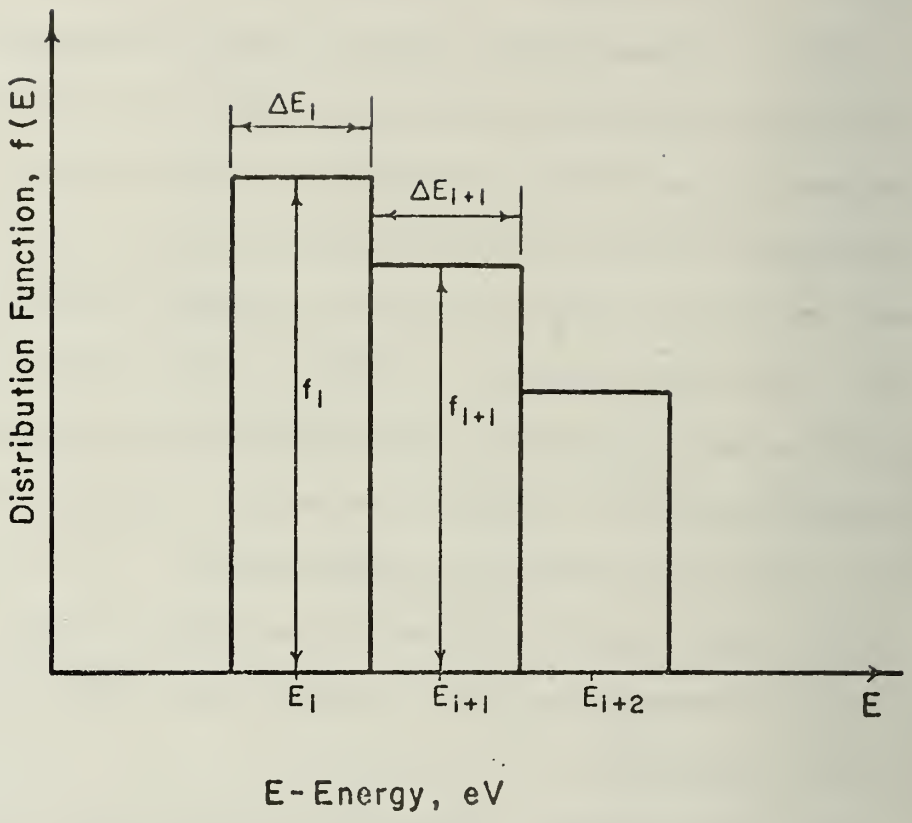


Figure 5. Rectangular block representation of the electron energy distribution histogram.

$$\frac{\Delta\bar{E}_i}{\Delta E_i} = \frac{\Delta f_i}{f_i}$$

or $$\Delta f_i = f_i \frac{\Delta\bar{E}_i}{\Delta E_i} \qquad (62)$$

where $\Delta\bar{E}_i$ is the deviation of the average energy $\bar{E}_i$ from E_i or $\Delta\bar{E}_i = \bar{E}_i - E_i$. Also Δf_i is the corresponding deviation of the frequency distribution at location index i.

Equation (62) provides a relative measure of the amplitude of the deviation of density distribution curve at energy E_i which can be used for comparing the efficiency of different variance reduction techniques as well as provide an heuristic clue to the modification of the fitted density distribution curve.

2. Data Filtering

The random errors (statistical fluctuations) result in bumps and ridges in the estimated frequency distribution function. It may be possible to alleviate many of these distortions by means of data smoothing techniques (data filtering).

Two types of data smoothing techniques commonly used in the processing of time series might be used here:

a. Moving averages - this technique operates by replacing each point of the frequency distribution function (height of the histogram at $E_i V_i$) at time cycle t_j with an average value of several subsequent points in the time cycle series. Thus if f_{ij} is the value

of frequency function at ith energy interval and jth time cycle, then f_{ij} is replaced by

$$\sum_{j=1}^{M} f_{ij} \cdot W_j / M$$

where W_j, the weighting factor for the jth time cycle, usually has the value of 1 or we can define it as a function of Δt_j. The value of M is the number of successive points of the time cycles to be included in each average.

b. Parabolic filtering - this is similar to the moving averages technique, but M is selected as an odd number, the point to be replaced is located in the center of these M points, and a parabola is fitted to these points by means of least squares. Thus it is replaced by the corresponding point f_i on the derived parabola. The process is repeated by shifting the center point to the next one in the time cycle series.

The technique of moving averages (a) is employed in the program, because of it's simplicity and the fact that the parabolic smoothing technique is too sensitive to the changes in the distribution function. Note that this smoothing (filtering) technique only becomes effective as the simulated system reaches steady state.

C. Solutions of the Problem

1. Preliminary Checks

In order to verify that the model is valid and correctly working, and the computer program is free of bugs, blunders, and systematic errors, we solved a specific problem first reported by J. A. Smit (11) and later extended by Heylen and Lewis (10). Their solutions for the electron energy distribution were obtained analytically based on the Boltzmann transport equation for the special case characterized as follows:

i) electric field present

ii) no external sources

iii) infinite size medium of background noble gases.

The comparisons are made for helium gas at $E_{f/p}$ = 4, 5, 10 V/cm^{-1}. ($E_{f/p}$: electric field strength to pressure ratio). The results are shown in Figures 6, 7 and 8. Both Smit and Heylen's results have taken into account all the collision processes including those due to elastic loss as well as inelastic losses. Heylen's results is more up-to-date, for low $E_{f/p}$ values only $E_{f/p}$ = 5 is given, which was chosen for the present comparison. In so far as possible, the same cross sections as Smit and Heylen and Lewis used were incorporated in the present calculations. The slight discrepancies apparant at the low-energy end is probably due to differences in treating the scattering process, and

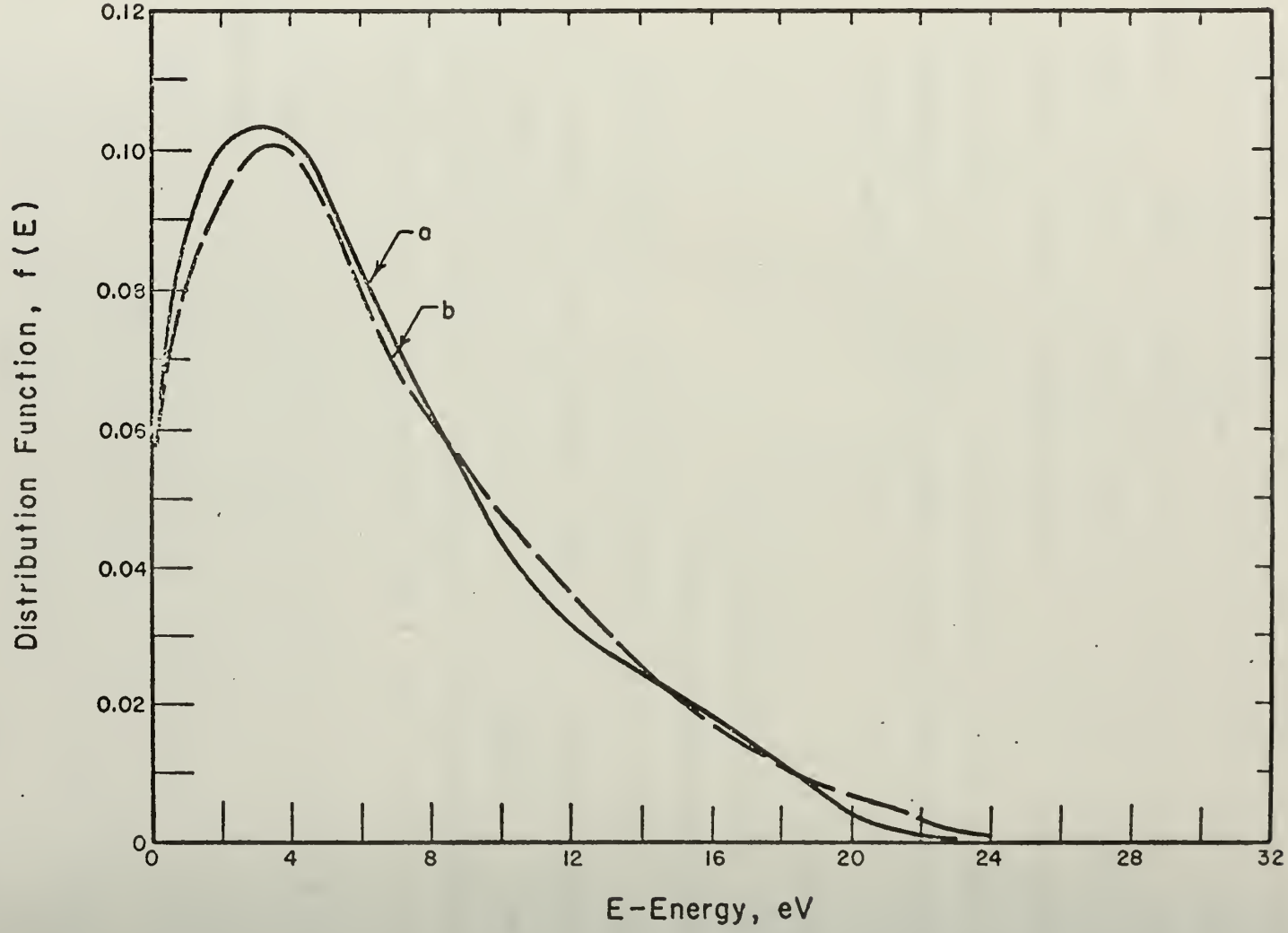


Figure 6. Comparison of the electron energy distribution for He at $E_{f/p} = 4$ for
a) Smit's calculation (1936) ($\bar{E} = 6.4$)
b) present calculation ($\bar{E} = 6.51$)

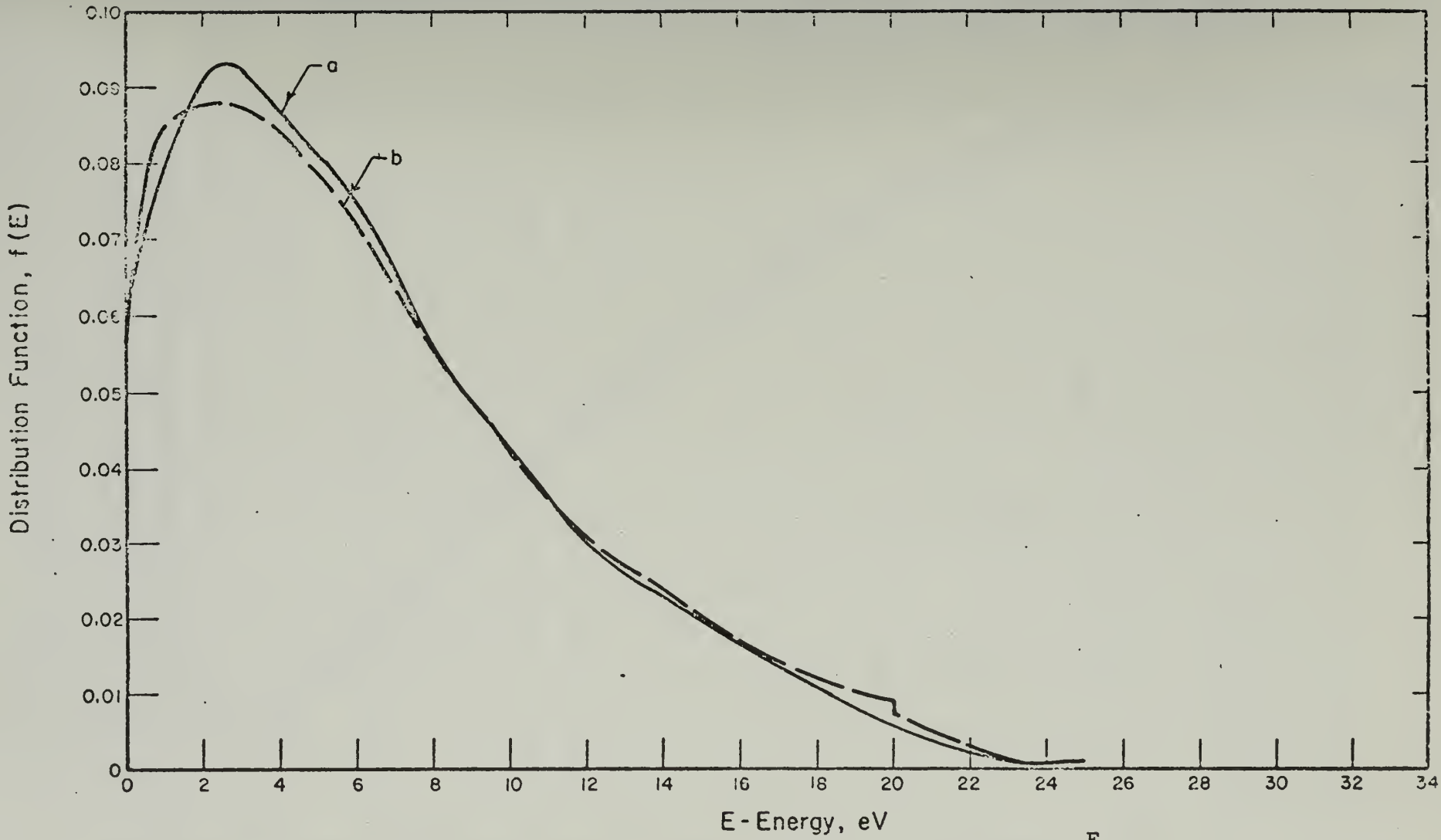


Figure 7. Comparison of electron energy distribution for He at $E_{f/p} = 5$
a) present calculation ($\overline{E} = 6.64$)
b) Heylen and Lewis' result ($\overline{E} = 6.51$)

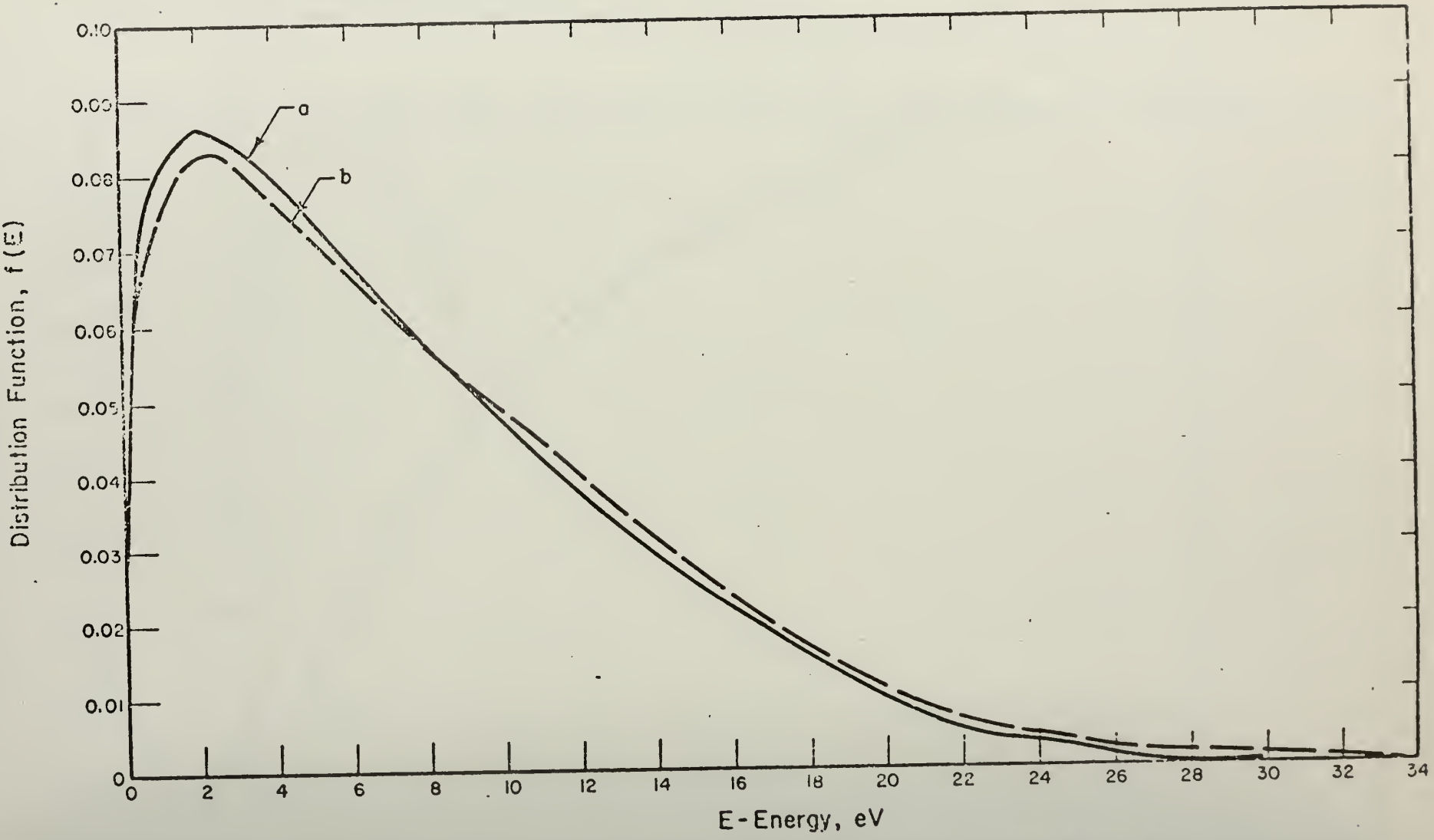


Figure 8. Comparison of electron energy distribution for He at $E_{f/p} = 10$
a) Smit's result ($\overline{E} = 7.7$)
b) present calculation ($\overline{E} = 7.83$)

the many approximations required in their analytic solutions. Also, some of the cross sections used in this calculations are experimental values, which may differ by some amount from that used for analytic solutions.

For the high energy region (near the source energy) checks have been made against the analytic solutions reported by Lo and Miley (32). As shown in Figure 9, the general shape of the electron energy flux distributions are in reasonable agreement. In this case it was not practical to use the same cross sections as incorporated in the analytic solutions, and this may account for some of the differences observed. Also the analytic solutions are obtained for an infinite medium vs. a 1 cm slab in the present case. Thus the analytic solutions do not allow leakage, although this becomes important in the present calculation for low pressures. Lo and Miley's results are plotted in Figure 9 for the source energy E_0 = 1500 eV and E_0 = 500 eV, whereas the present results are for E_0 = 1000 eV. The plot shown is for the flux density (normalized) instead of energy number density. They are related as follows:

$$\varphi(E) = f(E) \cdot V(E) \tag{63}$$

where $\varphi(E)$: electron flux density

$f(E)$: electron number density

$V(E)$: Electron kinetic velocity

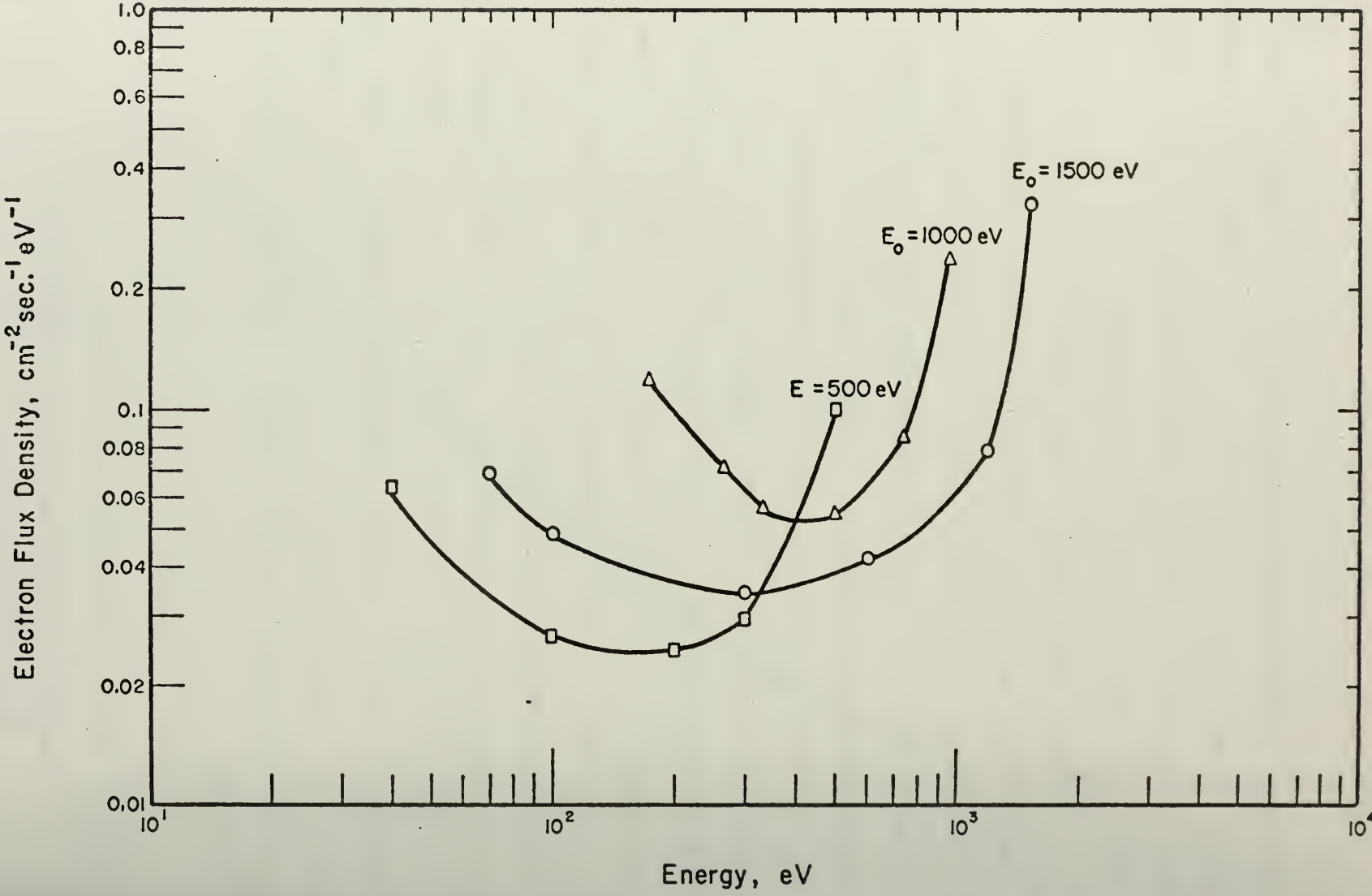


Figure 9. Comparison of the high-energy portion of flux density curve
a) E_0 = 1500 eV and E_0 = 500 eV: Lo and Miley's result

Since we only intend to compare general shapes of distribution, the normalizations used for the various curve, shown here are arbitrarily choosen for optimum display of information.

2. The Electron Energy Distribution Function without Electric Field

The calculations for electron energy distribution functions for helium with a high energy electron source, but no applied electric field (Figures 10 to 14) were carried out at two different pressures and various source rates. The slab thickness D is chosen to be fixed at D = 1 cm, which is equal to the actual diamter of cylindrical tube used in the laboratory (7). The two pressures are chosen to be P = 10 torr and P = 760 torr, corresponding to a typical low-pressure case and a normal atmospheric pressure.

We have chosen two different source energies (E_0), one at E_0 = 1,000 eV and the other at E_0 = 70 eV. These values roughly correspond to the highest energy and the average energy in the primary electron energy spectrum for MeV alpha-particle irradiation of helium as done in the experimental studies conducted at the University of Illinois (6).

The range of interest for the source rates for a boron coated tube irradiated in the Illinois TRIGA reactor lies between 10^{14} to 10^{18} (#/cm^3-sec). However, results shown for source rates above about 10^{16} are questionable since the resulting ionization density becomes large enough that

electron-electron collisions become important, and this process was neglected here.

The major quantity of interest here is the electron energy distribution function which were defined as $\bar{n}(E)$ in Chapter II. For simplicity, we represent the normalized distribution corresponding to $\bar{n}(E)$ by f(E). This normalization is defined by:

$$\int_{o}^{E_o} f(E)\, dE = 1 \qquad (64)$$

For the plasma system without electric field ($E_f = 0$), the distribution functions with source energy $E_o = 1000$ eV are shown in Figures 10 and 11 for the pressure p = 10 torr, and p = 760 torr respectively. Similar distribution functions for $E_o = 70$ eV are shown in Figures 12 and 13.

An idealized Maxwellian distribution plus 1/E tail are shown in Figures 10 to 13 for reference. (The Maxwellian plus 1/E distribution was used as the initial distribution for these calculations. Note that since this curve is for reference only, it is arbitrarily normalized to a point on the Maxwellian curve and does not satisfy Equation 64.) For the range of source rates mentioned, the calculated energy distribution for helium (He) are reasonably Maxwellian at low energy region. The differences due to variations in the source rates show up at the high energy end, especially near the source energy, where the magnitudes seem to depend linearly on the values of source rate. This is somewhat

deceptive, however, since the absolute magnitude at any point is due to the normalization. (This point is stressed again later in connection with Figure 24).

The fact that the distributions drop off rapidly for energies above about 20 eV is attributed to the fact that the threshold energy for inelastic processes is 20 eV, above which energy the ionization and excitation processes bring more electrons into the low-energy region.

In order to investigate the change in distribution function at very high source rates, a calculation for S_o = 10^{22} particles/cm^3-sec was carried out. As mentioned earlier, the neglect of electron-electron collisions makes the accuracy of this calculation questionable. Still the trends are of interest, and it is seen from Figure 14 that the distribution curve changes drastically. In fact, it is no longer Maxwellian at the low-energy end. Due to the high source rate, more high-energy particles and more particles with energy in the range from 0.3 eV to 20 eV are present in the system.

As discussed earlier, the distribution curve drops sharply for energies above the excitation threshold energy (at E = 20 eV) due to the dominance of ionization and excitation collision processes. At the higher pressure, the distribution curves decrease more rapidly compared to low pressure, since increased scattering slows the electrons down more rapidly. This effect is shown in Figures 15 and 16,

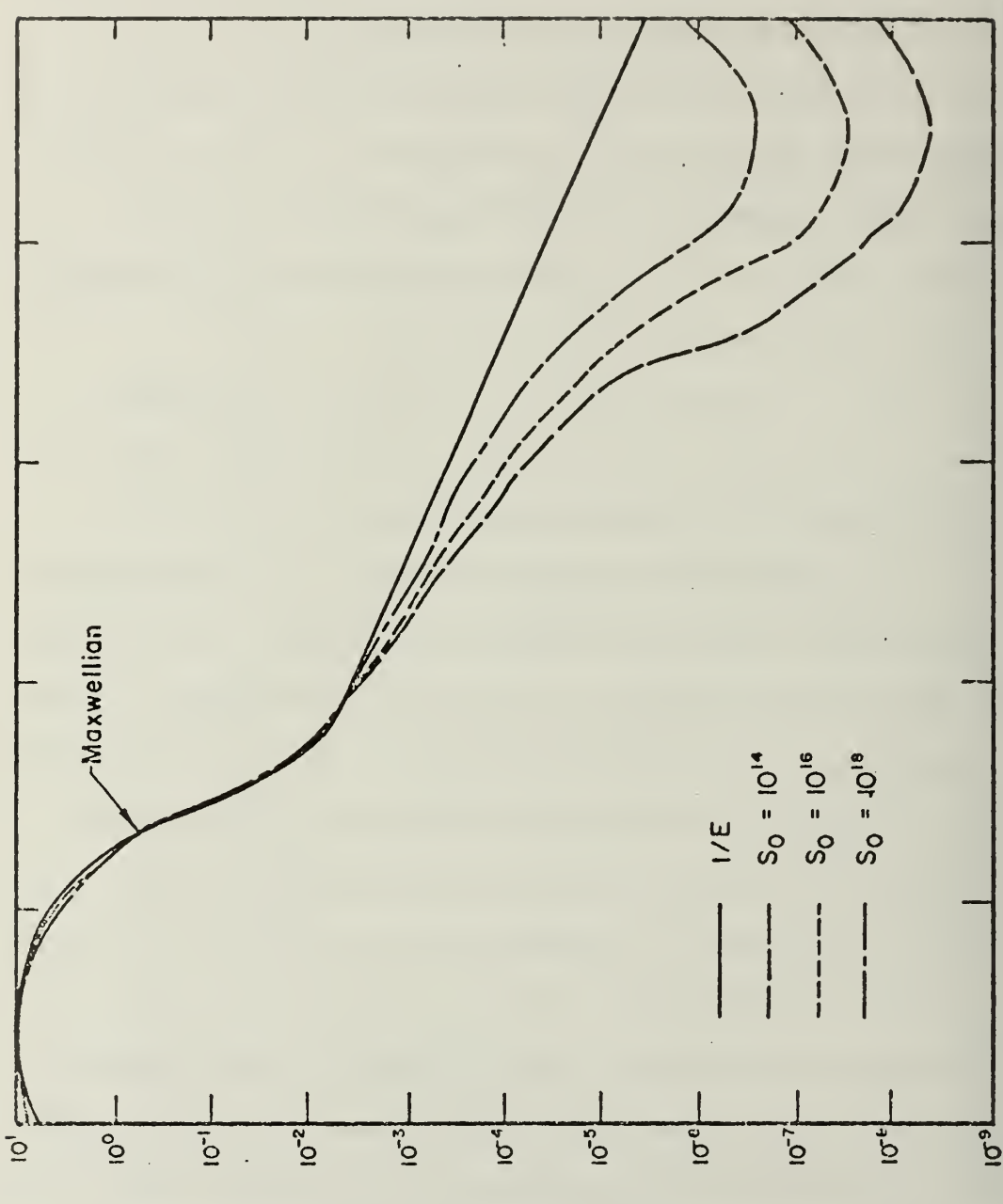


Figure 10. The electron energy distribution for He without an electric field but different source rates at p = 10 torr, E_o = 1000 eV and

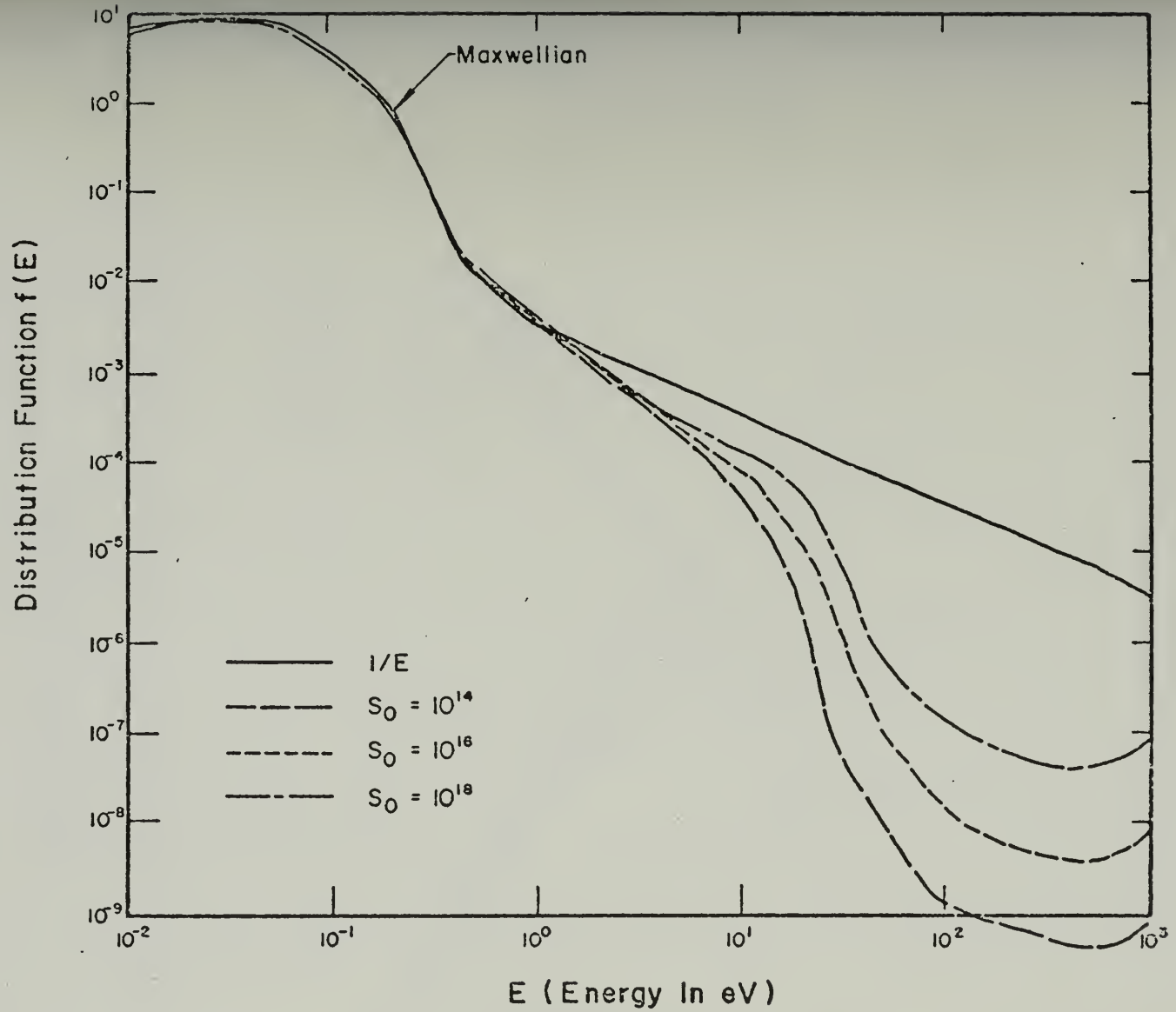


Figure 11. The electron energy distribution for He without an electric field but different source rates at p = 760 torr, E_0 = 1000 eV and Maxwellian plus 1/E distribution.

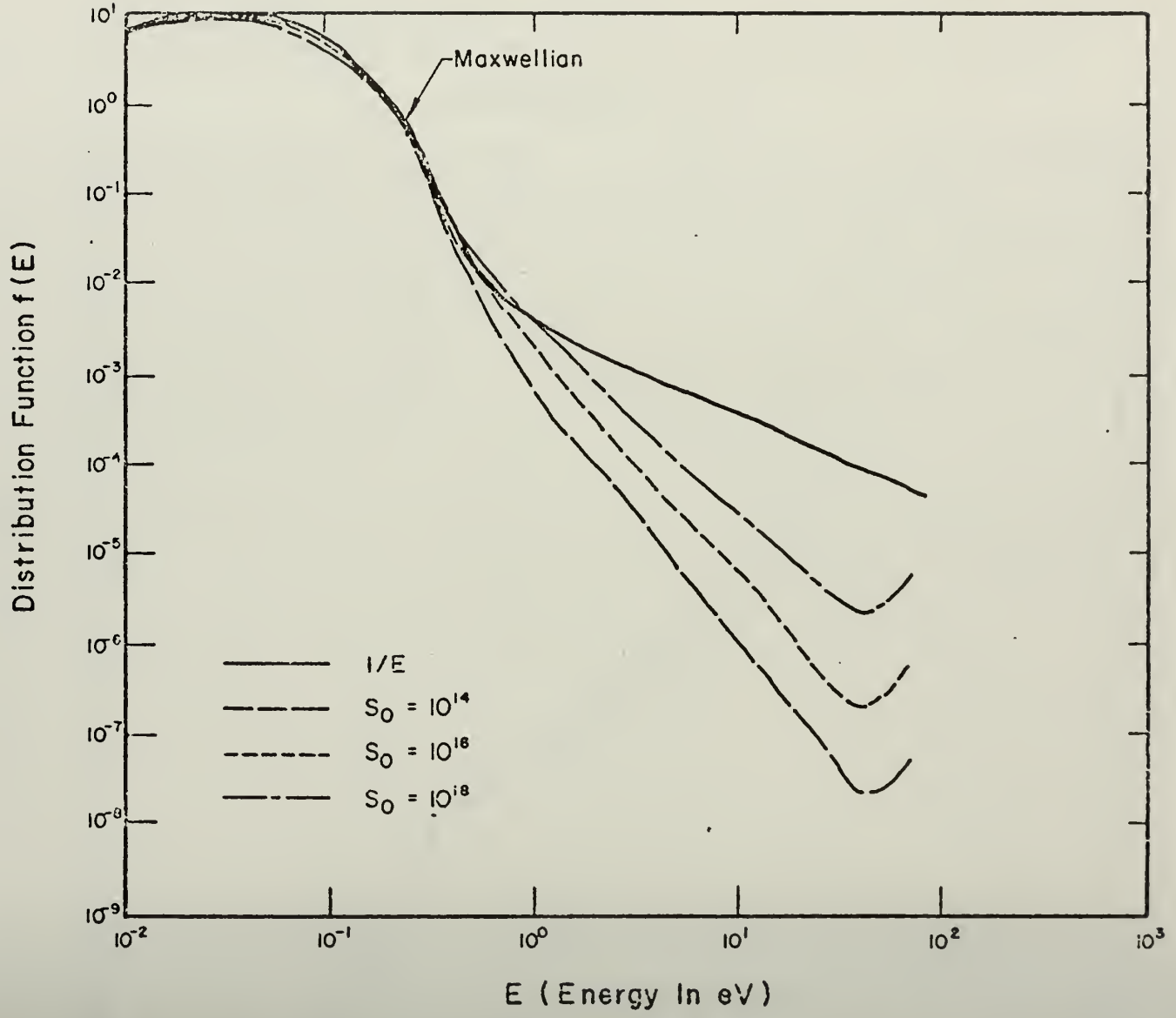


Figure 12. The electron energy distribution for He without an electric field but different source rates at p = 10 torr, E_0 = 70 eV and Maxwellian plus 1/E distribution.

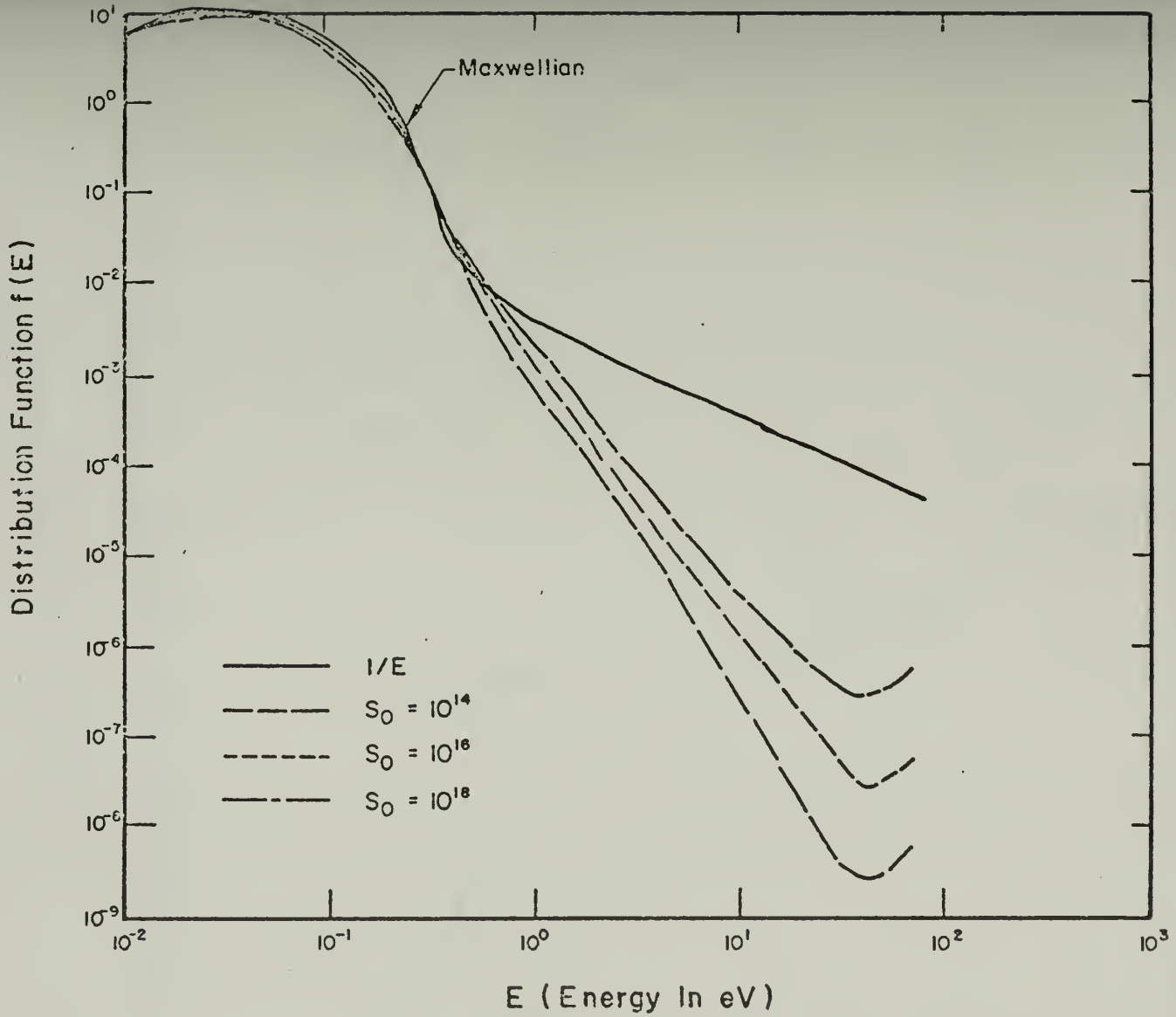


Figure 13. The electron energy distribution for He without an electric field but different source rates at p = 760 torr, E_0 = 70 eV and Maxwellian plus 1/E distribution.

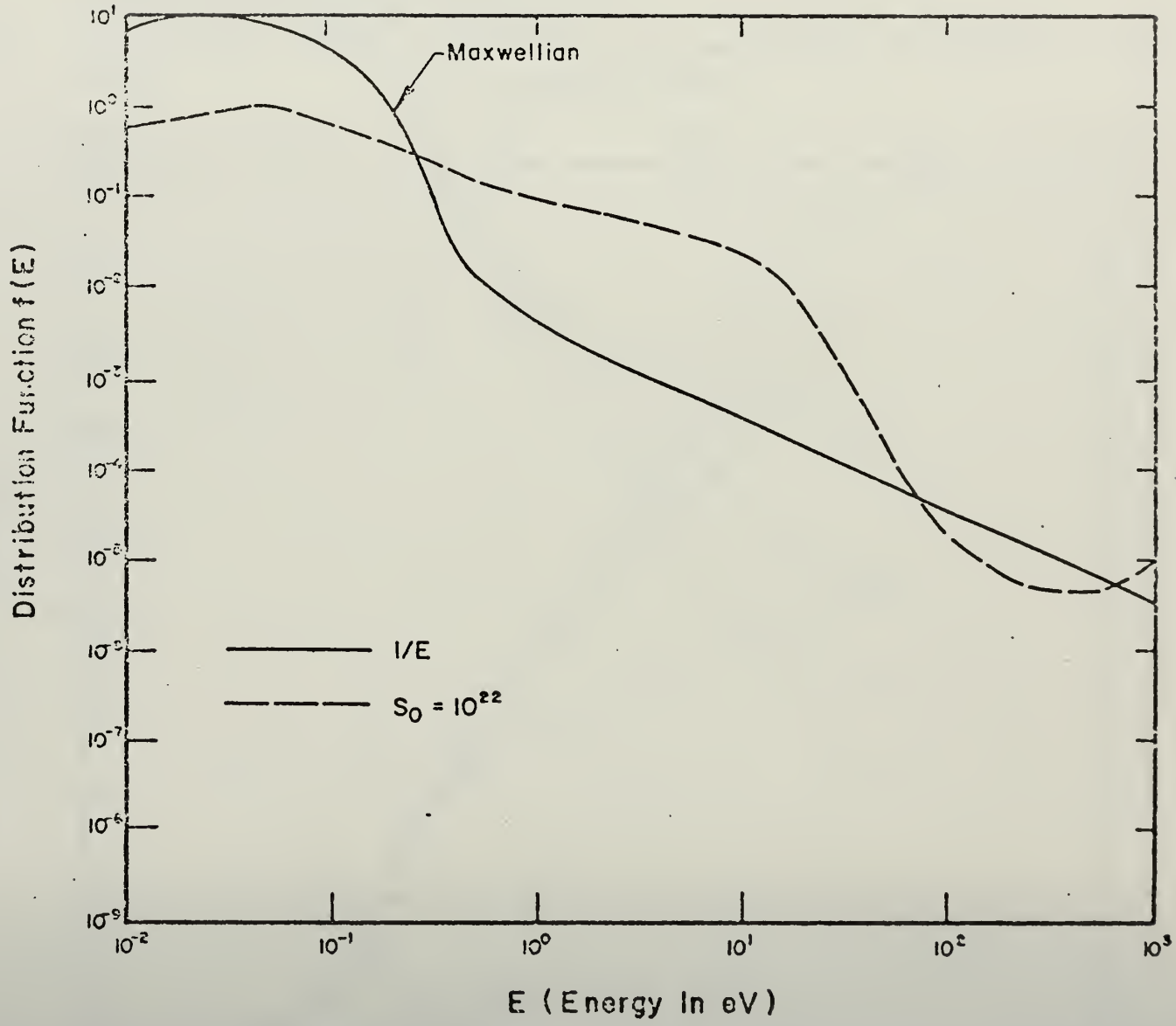


Figure 14. Comparison of f(E) for He without an electric field (source rate S_o = 10^{22} #/cm^3-sec) with the standard Maxwellian distribution plus 1/E tail.

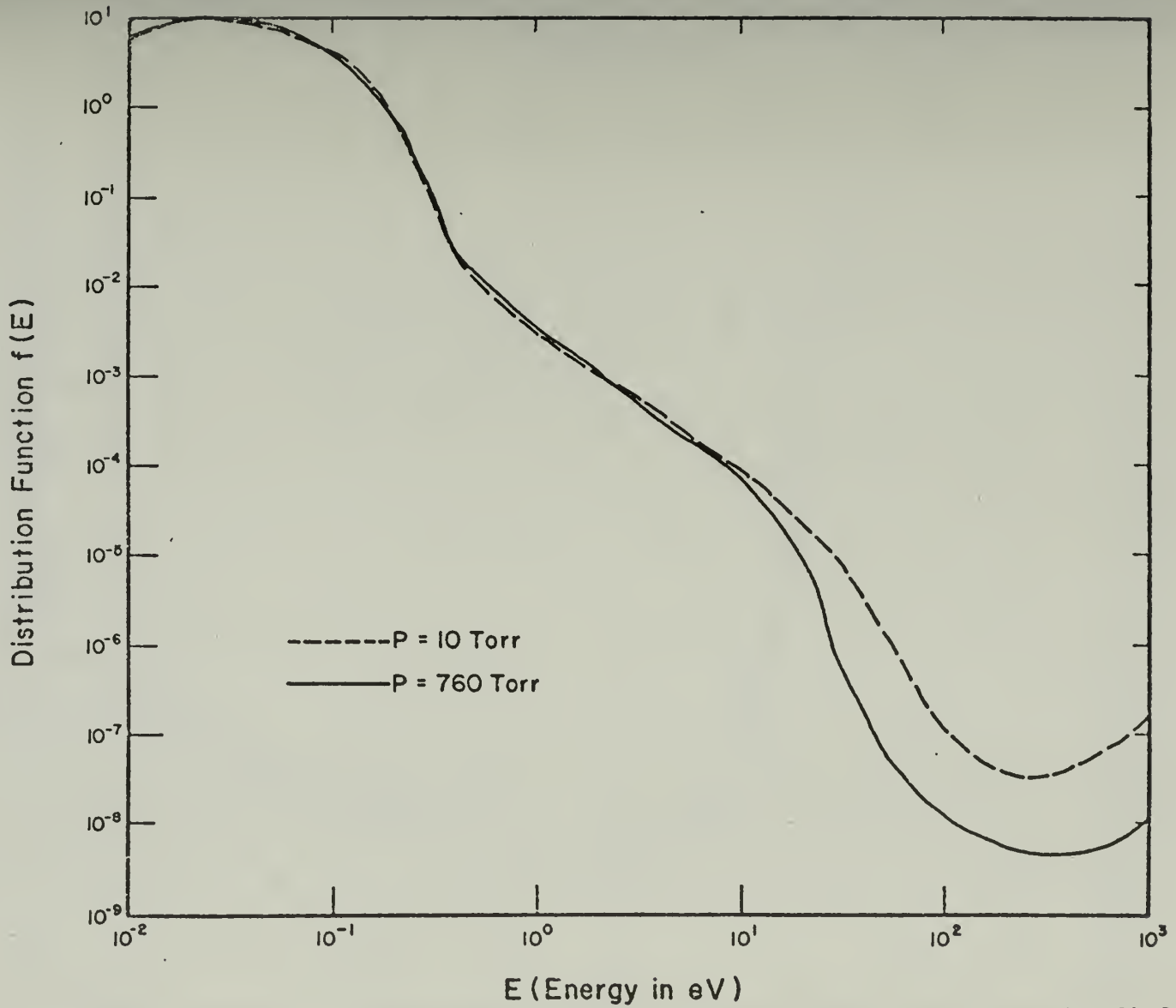


Figure 15. The electron energy distribution for He, without an electric field, for different pressure at $S_o = 10^{16}$, $E_o = 1000$ eV.

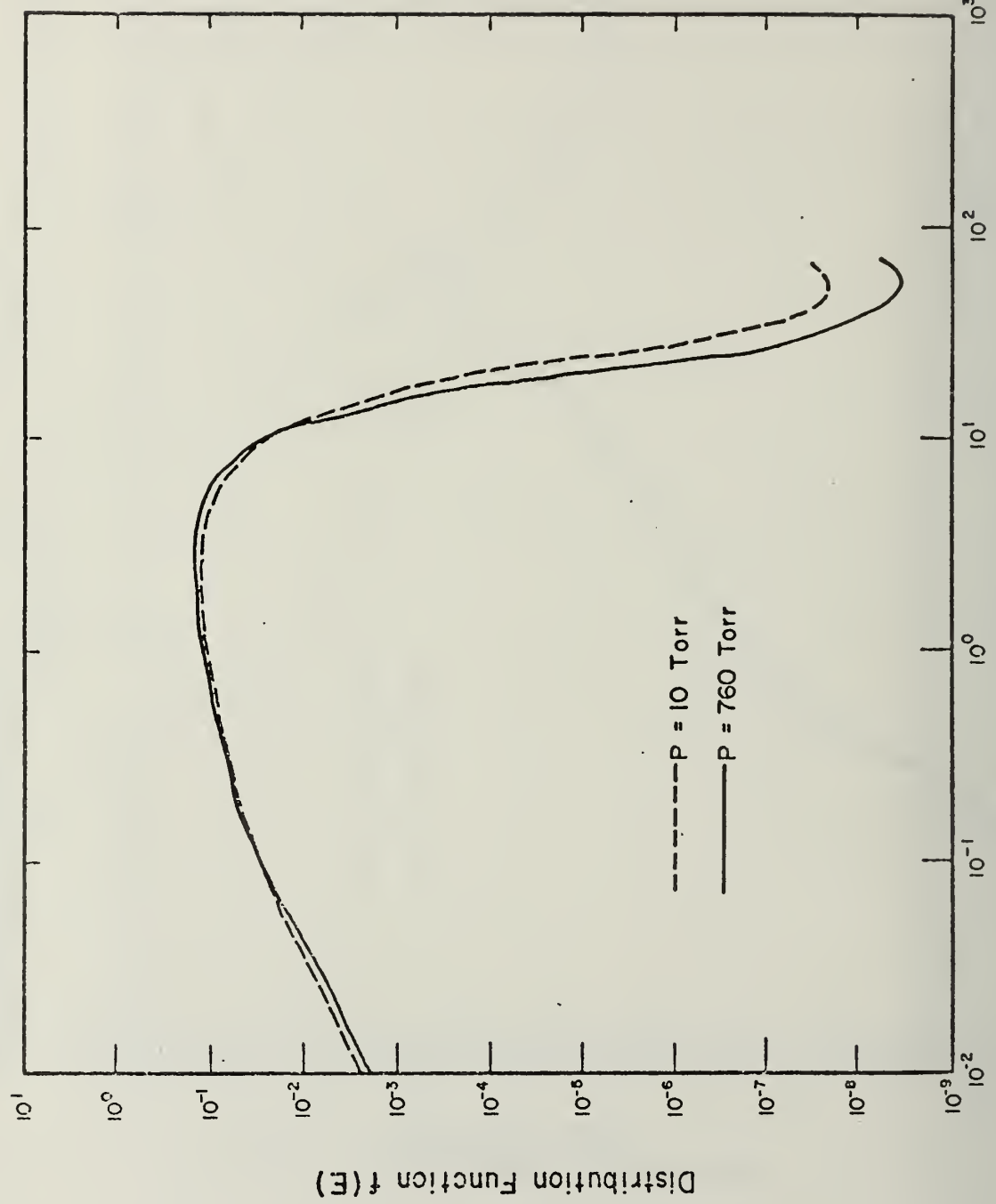


Figure 16. The electron energy distribution for He, without an electric field, for different pressure at $S_o = 10^{16}$, $E_o = 70$ eV.

for the same source rate $S_o = 10^{16}$ (#/cm^3-sec) and source energy, but two different pressures. The reduction in magnitude of the high energy tail as the pressure increases is clearly illustrated.

In these calculations, the rate of both leakage and absorption (recombination) are strongly dependent on the pressure. At higher pressures (e.g., p = 760 torr), very few particles leak out of the system, and the loss are dominated by the absorption process. For lower pressure (p = 10 torr), fewer particles are absorbed, while more escape or leak out of the system. Also, more particles escape in the high-energy region, but the absorped particles are mainly in the low-energy region.

The estimated major parameters are summarized in Table 1, which includes the average energy of the system ($\overline{E}$), the number of positive ions (N^+) and the W-values for various combinations of source rate S_o, source energy E_o and pressure p.

The W-value is defined as the amount of energy required (input) to produce an ionization pair (positive ion and electron), or

$$\text{W-value} = \frac{(N_s.E_o - E_{Tes} - E_{Tab})}{N_z} \qquad (65)$$

Where N_s: the number of source particles introduced into the system during the period Δt.

E_{Tes}: the total energy lost with escaping particles during the time Δt.

Table 1. Calculated Parameter Values for the Plasma Without a Electric Field

* P (torr)	E_o (eV)	S_o (#/cm^3-sec)	$\overline{E}$ (eV)	N^+ (#)	W-value Range
10	1000	10^{18}	0.171	0.125×10^{14}	41 ~ 63
10	1000	10^{16}	0.157	0.125×10^{13}	35 ~ 53
10	1000	10^{14}	0.111	0.125×10^{12}	49 ~ 58
760	1000	10^{18}	0.167	0.583×10^{15}	32 ~ 38
760	1000	10^{16}	0.123	0.446×10^{14}	40 ~ 65
760	1000	10^{14}	0.104	0.67×10^{13}	35 ~ 54
10	70	10^{18}	0.104	0.125×10^{14}	50 ~ 62
10	70	10^{16}	0.082	0.125×10^{13}	47 ~ 63
10	70	10^{14}	0.075	0.124×10^{12}	40 ~ 57
760	70	10^{18}	0.082	0.16×10^{15}	47 ~ 65
760	70	10^{16}	0.075	0.141×10^{14}	42 ~ 58
760	70	10^{14}	0.075	0.157×10^{13}	39 ~ 55
Maxwellian distribution					
		0	0.05	---	---

*P: pressure, E_o: source energy, S_o: source rate, $\overline{E}$: average energy of the particles, N^+: number of positive ions.

E_{Tab}: the total energy lost with recombining particles during the time Δt

N_z: the total number of ionizations produced during the time period Δt.

As seen from Table 1, the average energy $\overline{E}$ tends to be higher for higher source rates and higher source energy, and it is lower for higher pressures. However, the differences are in general very small. (All the average energies are consistently greater than that of a Maxwellian distribution). The values for ion density N^+ are roughly proportional to the square root of source rate, and are higher for higher pressures, virtually independent of source energy.

The W-values are quite sensitive to statistical fluctuations, and the ranges of variation obtained over the last 10 time cycles in a given calculation are shown in Table 1. The W-values obtained here do not show any clear dependence on the system parameters, thus variation indicated may be totally due to the statistical fluctuations. This is not too surprising since the W-value is known to be roughly independent of particle energy, etc. The W-value for helium obtained experimentally by Jesse and Sadouski (34) is 43. A reasonable value to choose for the W-value from Table 1 would be 50, which is little bit higher than the experimental result. The reason for this discrepancy is not clear, but it may be due to small inaccuracies in the ionization-excitation cross section employed here. The W-value is, by definition, quite sensitive to the details

of the ratio of the ionization to the excitation cross section as a function of energy.

3. The Electron Energy Distribution Function with an Applied Electric Field

The calculated electron energy distribution functions in He with an applied electric field ($E_f/p = 10$) are plotted in Figures 17 to 21, in a manner similar to that in the previous section. All these calculations are carried out at the electric field to pressure ratio $E_f/p = 10$. Smit's result (without source or $S_o = 0$) are plotted together with present calculations at given pressure and source energy ($p = 10$, 760 and $E_o = 1000$ eV, 70 eV), with three different source rates. It is observed that the distribution functions are highly non-Maxwellian. For the source rate in the range 10^{14} #/cm^3-sec to 10^{18} #/cm^3-sec, the distribution curves at low energy end are quite close to the Smit's results (11). At the high energy end, they have a shape similar to the curves of no electric fields. Again differences due to the source rate show up at high-energy region. Below 10 eV, all the distribution functions fall on the top of each other, and they begin to spread out as the energy increases above 10 eV. For high pressures or low source energy, more difference (between $S_o = 0$ and $S_o \neq 0$) show up at high-energy end than that of low pressure and/or high source energy. Again at very high source rates ($S_o = 10^{22}$ #/cm^3-sec) the distribution function changes appreicably.

In Figure 21, the comparison is made with a very high source rate ($S_o = 10^{22}/cm^3$-sec) and with one in the region of interest ($S_o = 10^{16}$, p = 760 torr). For very high source rate, the distribution function changes quite a lot; it still preserves the general shape, but at low-energy end, it is much smaller in amplitude. (However, as stressed earlier, the high source rate calculation is questionable due to the neglect of electron-electron interactions.)

The changes in these distribution functions due to different pressures are also shown in Figures 22 and 23. The observed trends are similar to those in the previous section for the electric field $E_f = 0$ case.

So far, the normalized distribution functions f(E) have been displayed. However, to stress the fact that the absolute magnitudes of the curves depends strongly on the source (shapes have received our interest to this point), Figure 24 shows the unnormalized electron energy distribution functions for He (with electric field or $E_f \neq 0$) are plotted, with $E_f/p = 10$, p = 10 torr, $E_o = 1000$ eV, and three different source rates ($S_o = 10^{14}$, $S_o = 10^{16}$, $S_o = 10^{18}$). The magnitude (unnormalized) distribution is defined as

$$N^-(E) = N^+ \cdot f(E) \qquad (66)$$

where N^+: number of positive ions

f(E): normalized distribution

The values of N^+ are 0.24×10^{15}, 0.24×10^{14}, and 0.24×10^{13} corresponding to the three source rates $S_o = 10^{18}$, $S_o = 10^{16}$

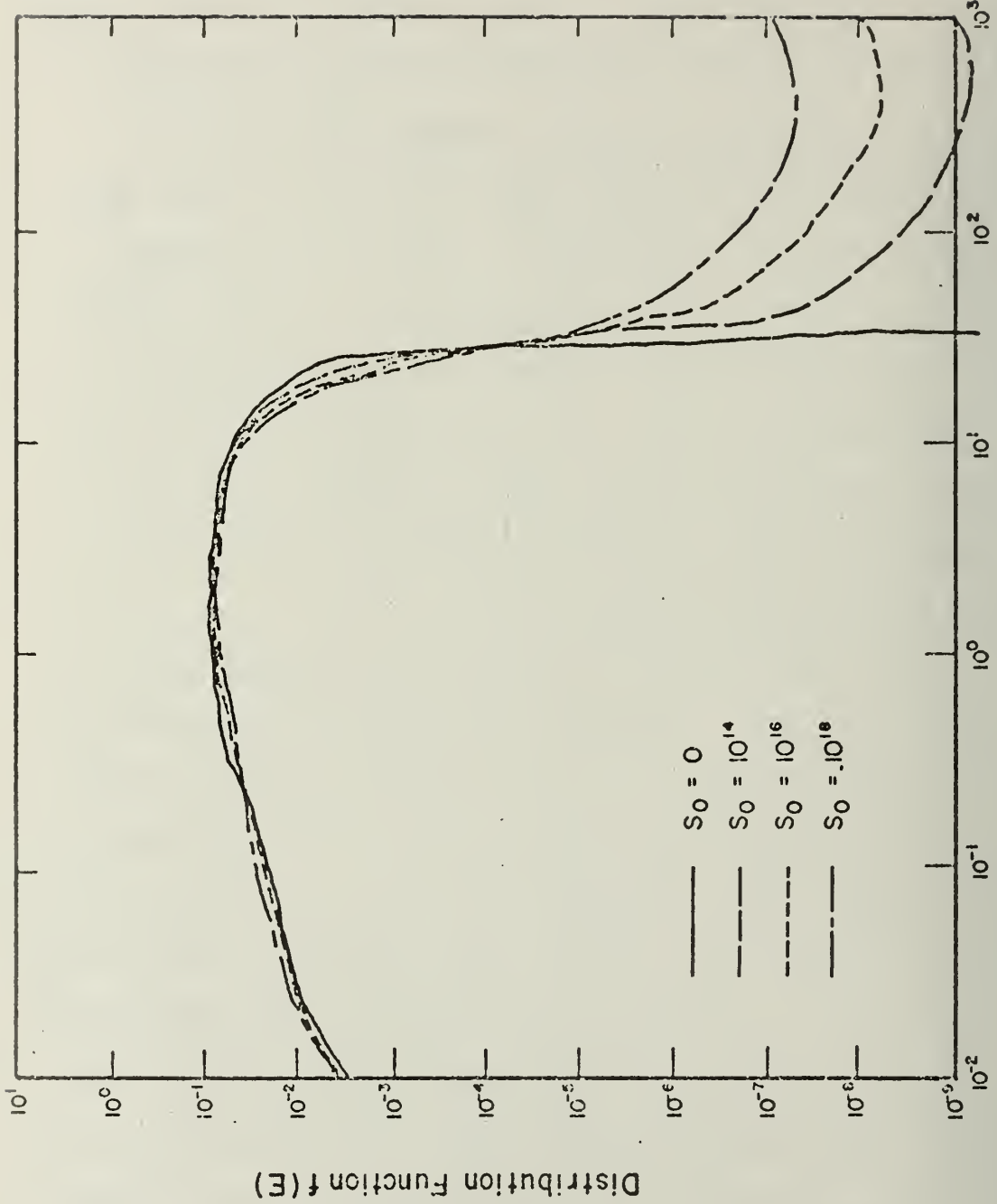


Figure 17. The electron energy distribution for He with an electric field at $E_{c/-} = 10$, p = 10 torr, E_0 = 1000 eV.

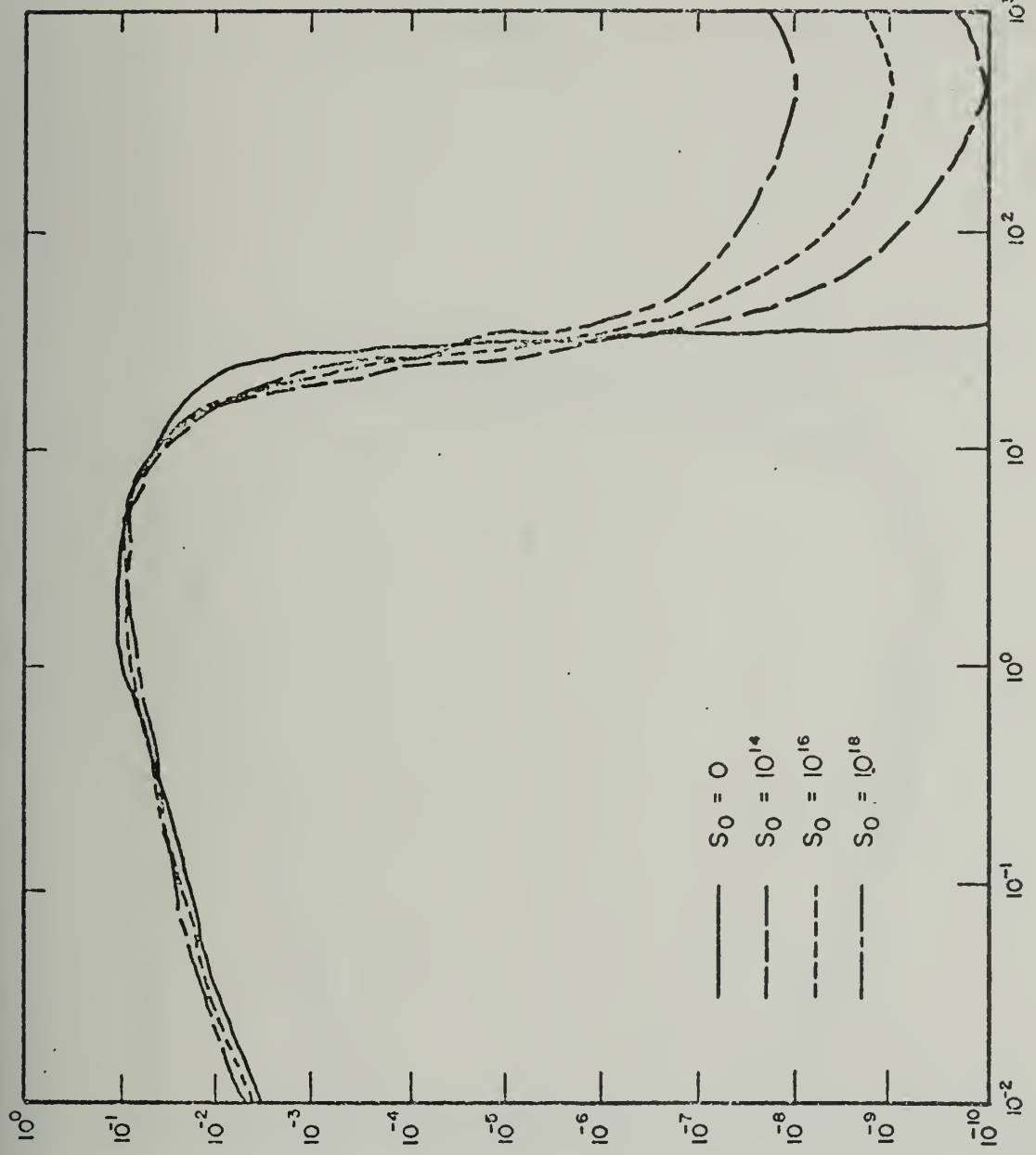


Figure 18. The electron energy distribution for He with an electric field at $E_{f/p} = 10$, p = 760 torr, E_o = 1000 eV.

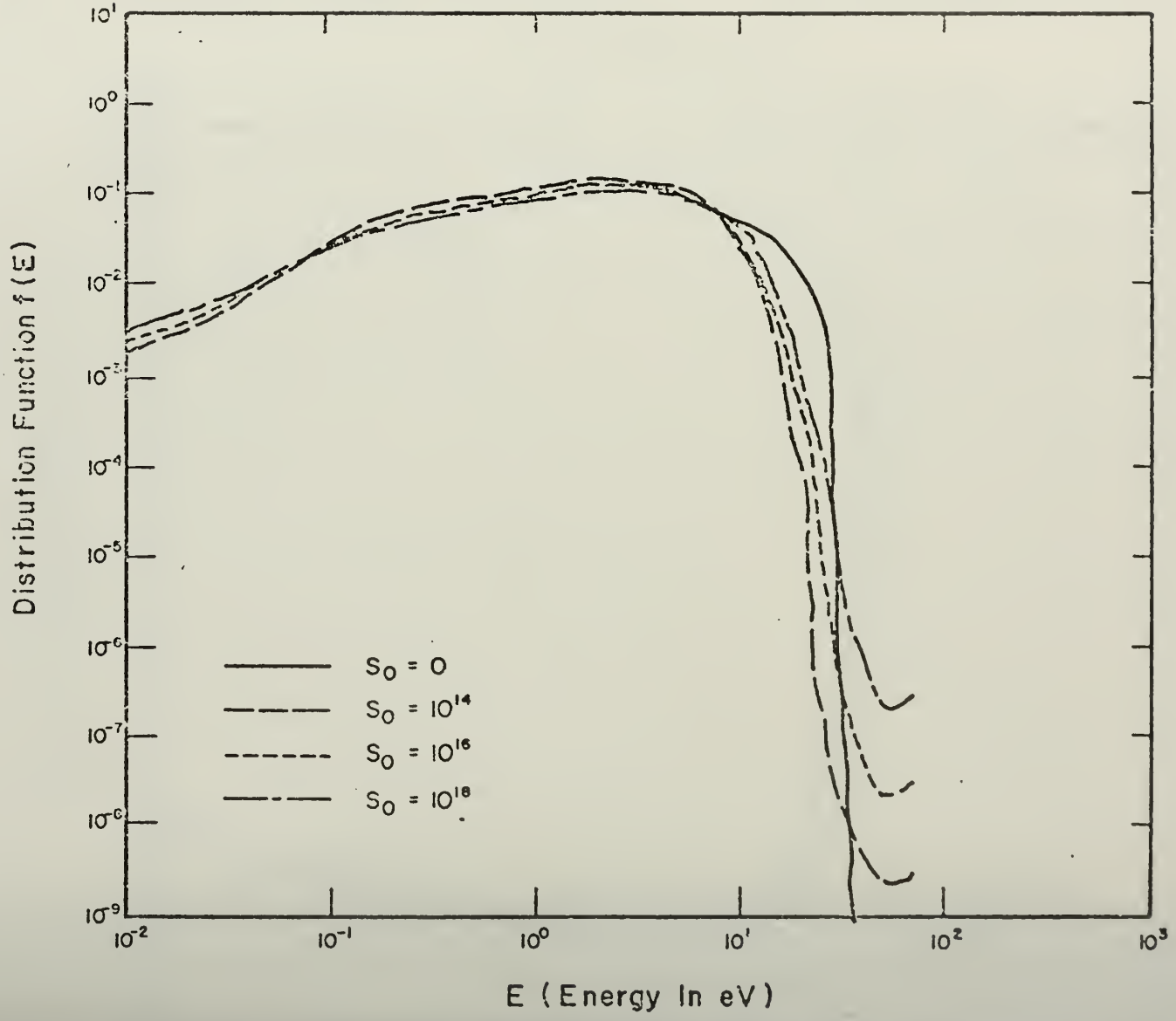


Figure 19. The electron energy distribution for He with an electric field at $E_{f/p}$ = 10, p = 10, E_o = 70 eV.

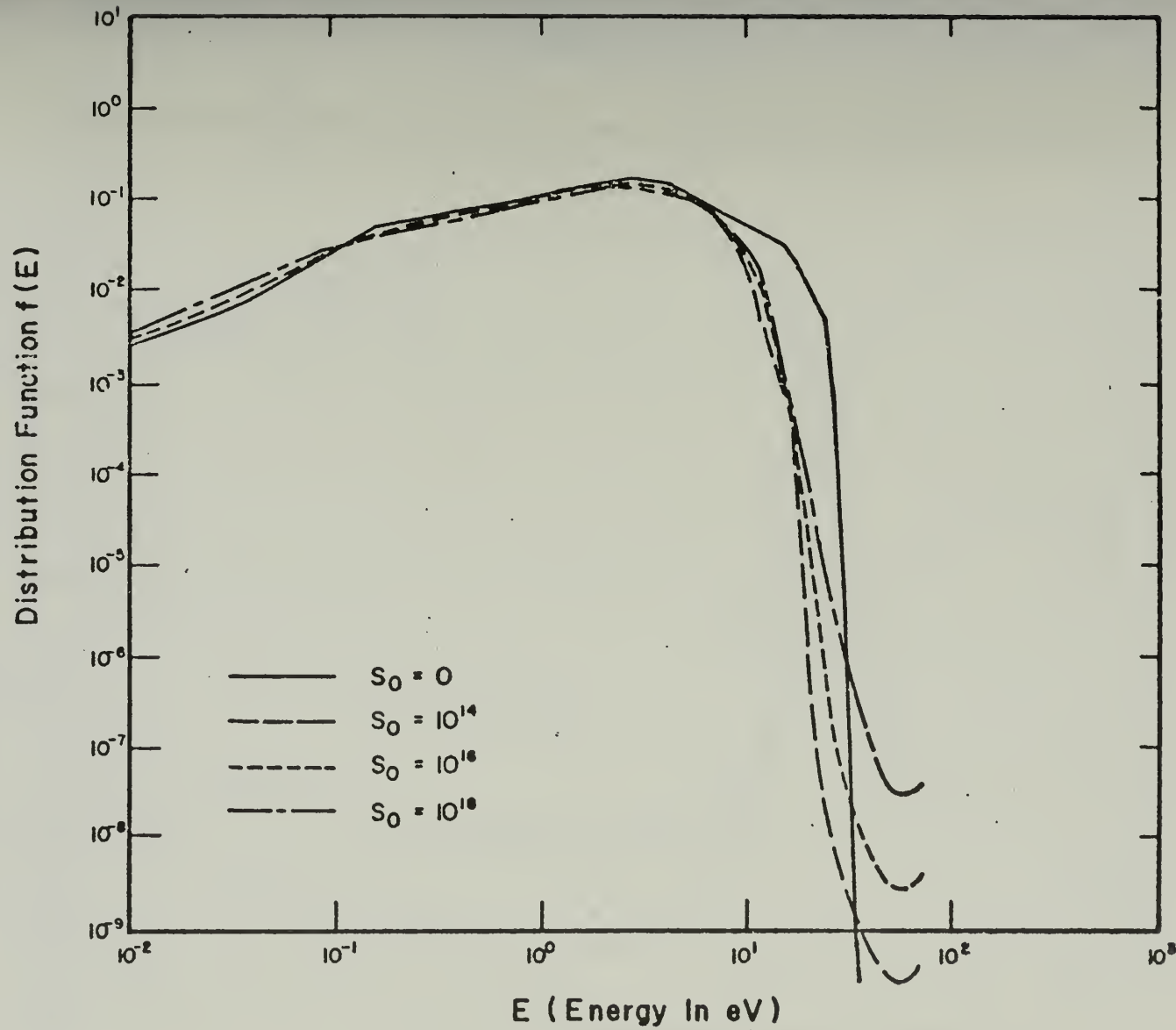


Figure 20. The electron energy distribution for He with an electric field at $E_{f/p} = 10$, p = 760 torr, $E_0 = 70$ eV.

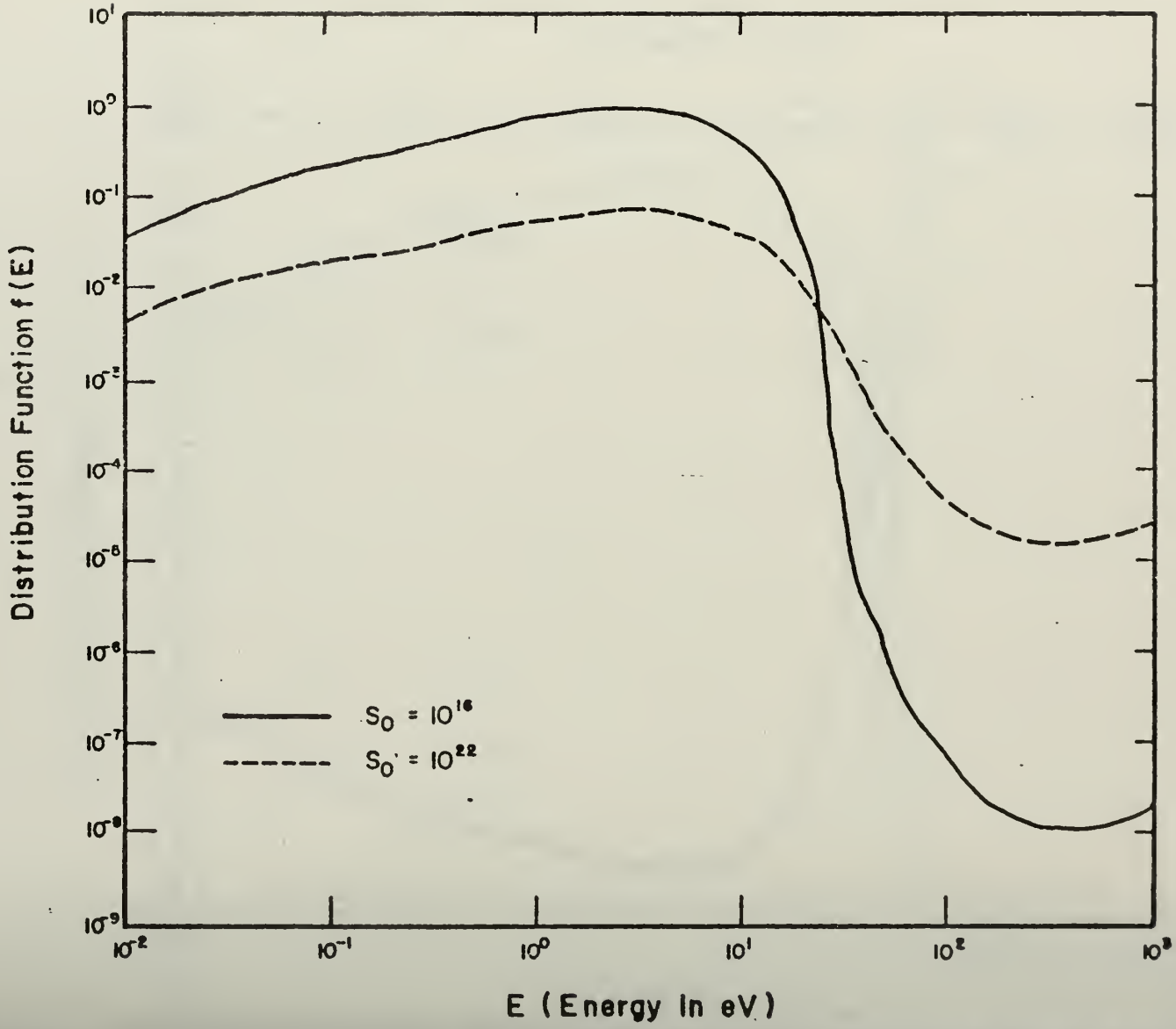


Figure 21. The electron energy distribution function at $E_{f/p}$ = 10, p = 760 torr for $S_o = 10^{22}$ and $S_o = 10^{16}$ (#/cm^3-sec).

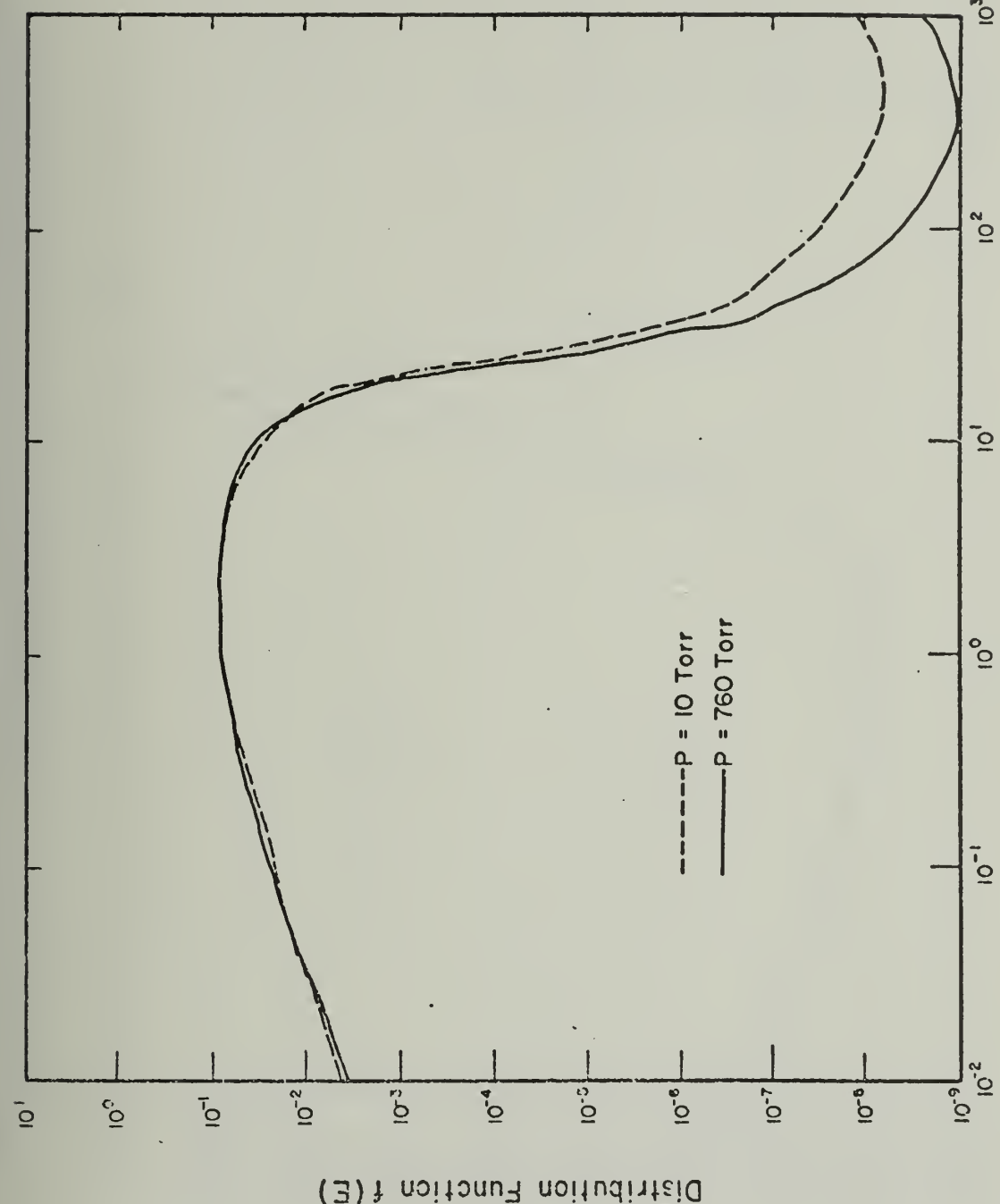


Figure 22. The electron energy distribution for He, with an electric field at $S_o = 10^{16}$, $E_o = 1000$ eV.

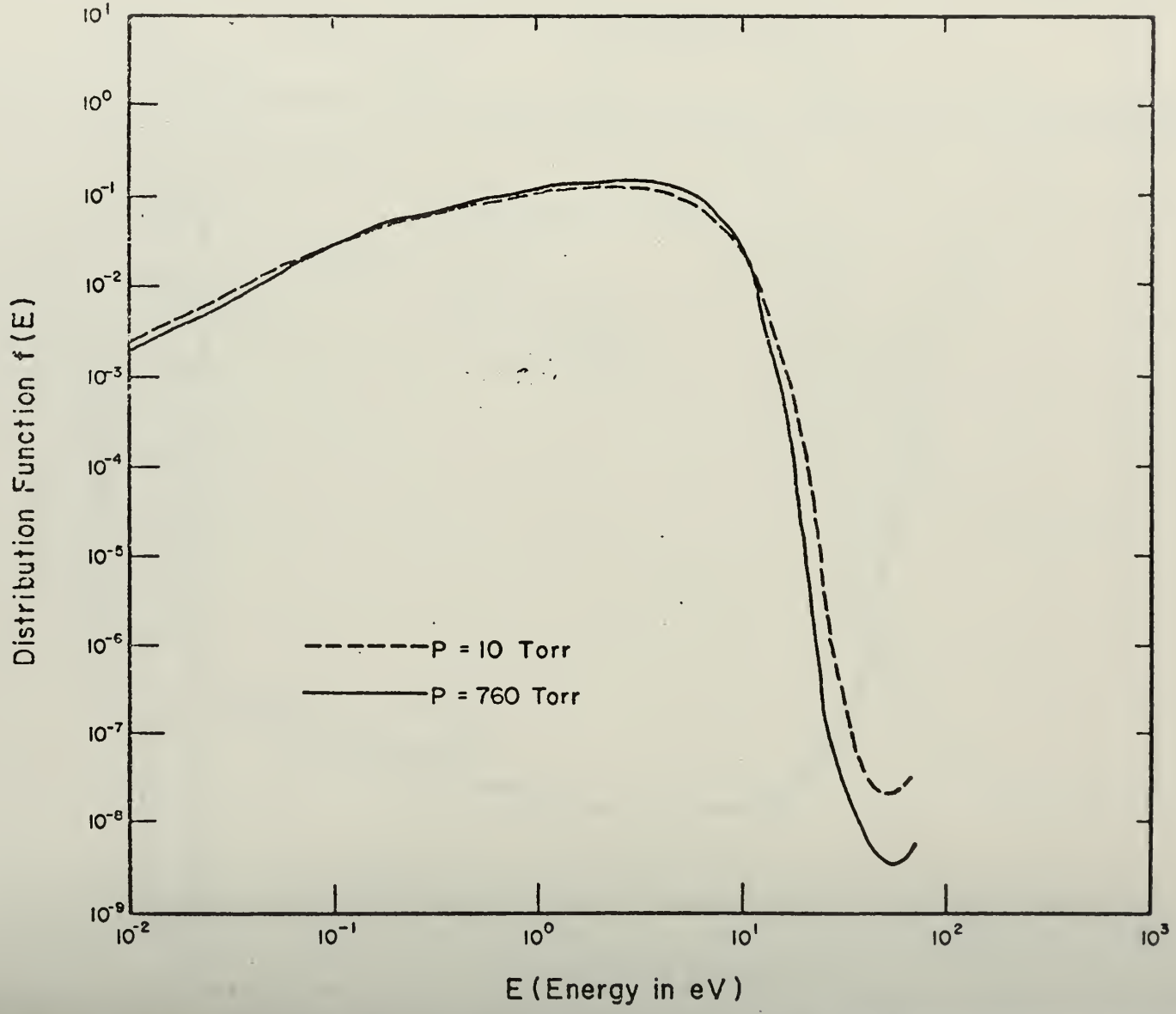


Figure 23. The electron energy distributions for He, with an electric field at

16,

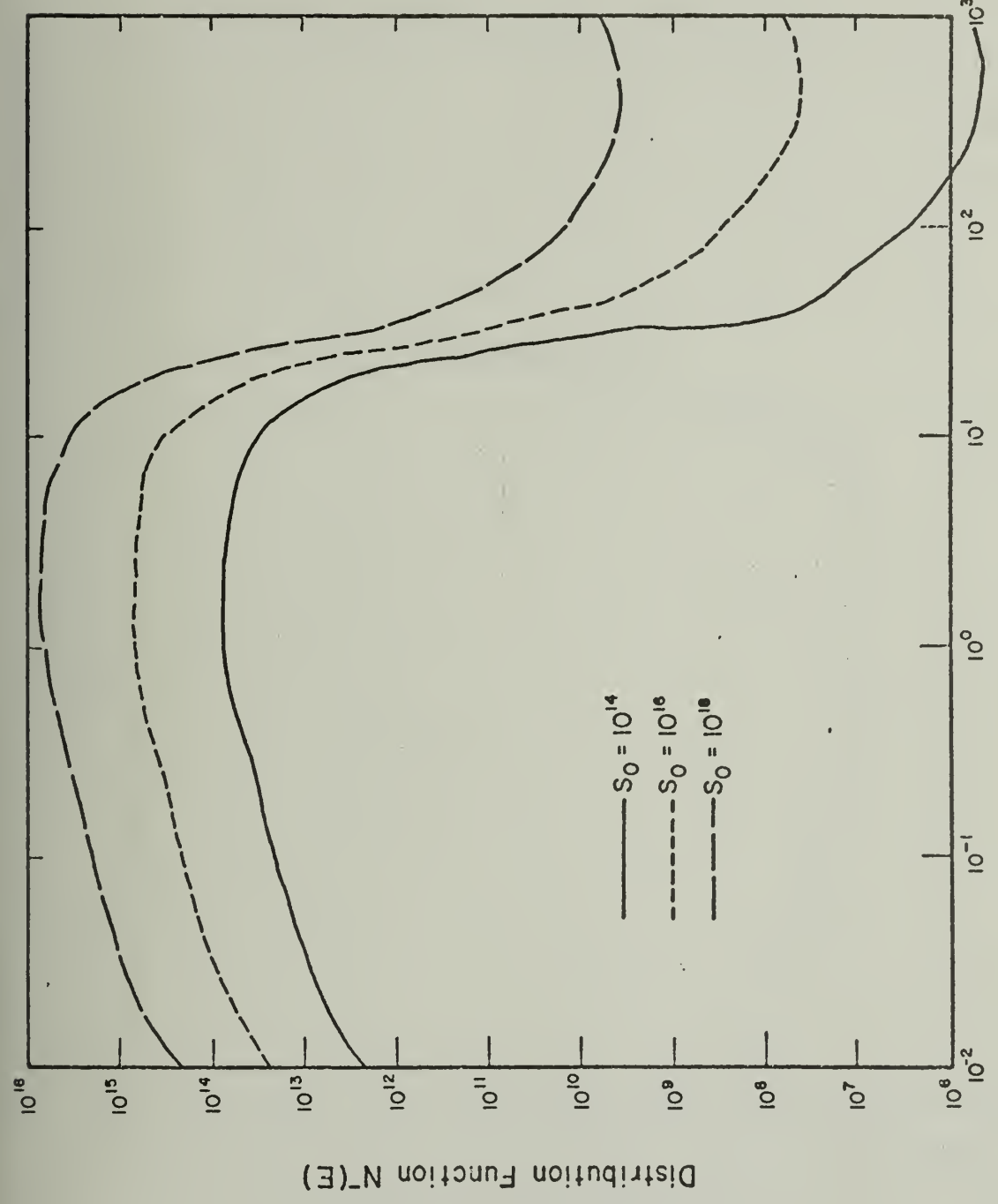


Figure 24. The unnormalized electron energy distribution for He at $E_{f/p} = 10$, p = 10 torr, $E_0 = 1000$ eV.

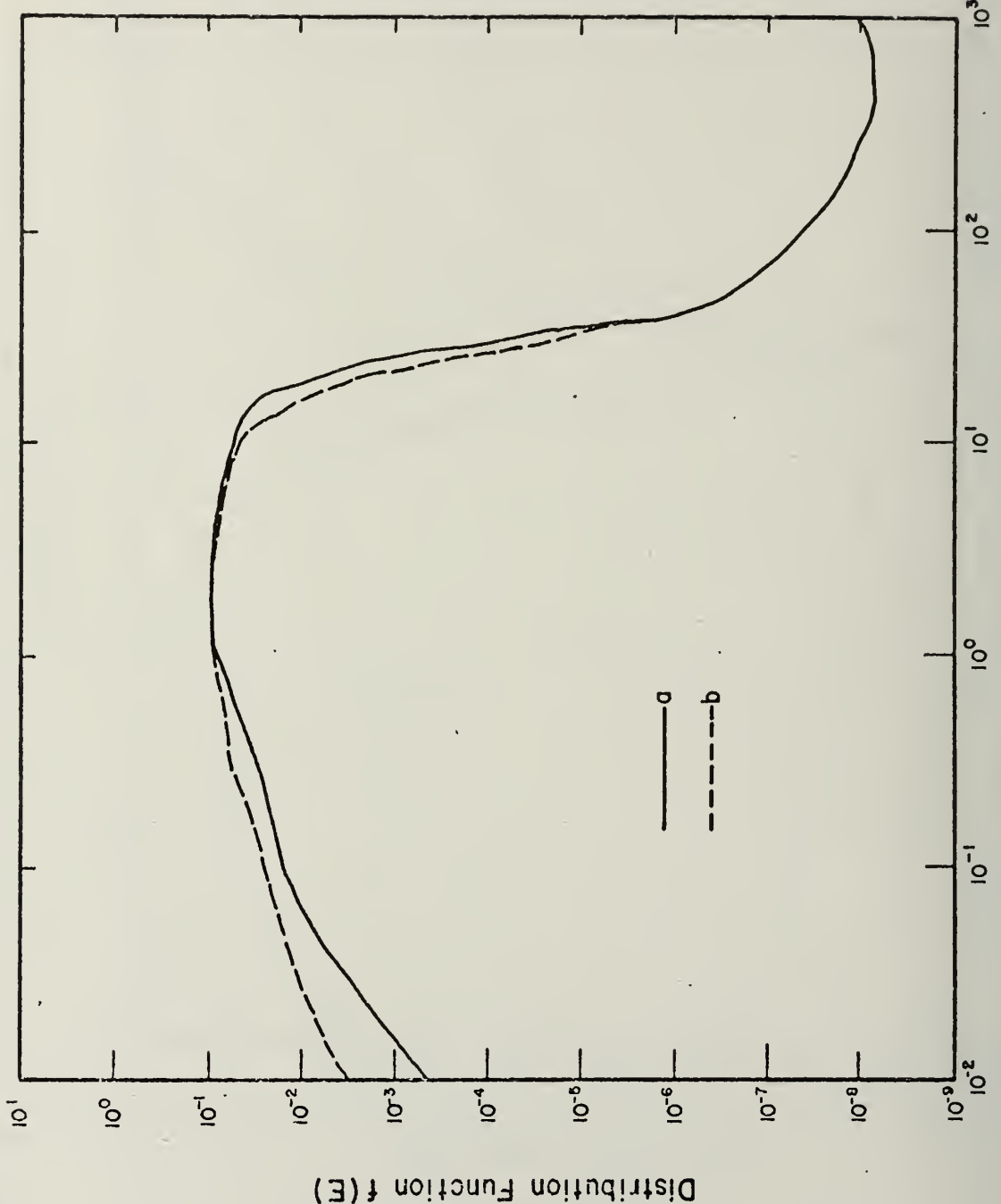


Figure 25. The effect of recombination on the electron energy distribution
a) with normal recombination cross section x 100
b) with normal recombination cross section x 1.

and $S_o = 10^{14}$, respectively.

In order to show the effect of recombination, a normal case is compared in Figure 25 to a calculation where the absorption cross section was arbitrarily increased 100 times. It is observed that the major effect comes in at low-energy region. More and more electrons recombine as they thermalize and hence, the lower energy region of the distribution is depleted. Since recombination does not occur at high energies, this region is not affected.

The calculated major parameter values for the system with an electric field are summarized in Table 2. As expected on physical grounds the values of the average energies for this case are much higher than the corresponding values with no electric field (compare to Table 1). However, other general trends are the same, e.g. the value of the average energies are slightly higher for higher source rate and/or higher source energy, but are lower for higher pressures.

For comparison the average energy (7.7 eV) found by Smit for an electric field and $E_{f/p} = 10$ but with no source present is included in Table 2. It is in general higher than the present values. The reason is not entirely clear. At first thought the additional high-energy source electrons might be expected to raise the average energy. However, as found by T. Ganley (37), the presence of high-energy electrons to produce ionization allows the electrons in the Maxwellian region to decrease in energy, and as a result the overall average may actually decrease.

Table 2. Calculated Parameter Values for Plasma with Applied Electric Field ($E_{f/p}$ = 10)

* P (torr)	E_o (eV)	S_o (#/cm^3-sec)	$\bar{E}$ (eV)	N^+ (#)	Modified W-value range
10	1000	10^{18}	8.1	0.24×10^{15}	35 ~ 44
10	1000	10^{16}	7.5	0.21×10^{14}	34 ~ 54
10	1000	10^{14}	7.3	0.24×10^{13}	37.5 ~ 60
760	1000	10^{18}	7.0	0.23×10^{17}	37 ~ 50
760	1000	10^{16}	6.6	0.204×10^{16}	30 ~ 51
760	1000	10^{14}	5.4	0.24×10^{15}	34 ~ 57
10	70	10^{18}	5.86	0.21×10^{15}	31 ~ 35
10	70	10^{16}	5.18	0.21×10^{14}	34 ~ 50
10	70	10^{14}	4.46	0.213×10^{13}	31 ~ 56
760	70	10^{18}	5.7	0.284×10^{16}	35 ~ 46
760	70	10^{16}	5.0	0.26×10^{15}	39 ~ 48
760	70	10^{14}	4.3	0.24×10^{14}	32 ~ 49
Smit's distribution					
		0	7.7	---	---

*p: pressure; E_o = source energy; S_o: source rate; $\bar{E}$: average energy; N^+: number of positive ions.

The values of N^{+} are roughly proportional to the square root of the source rate (recall Equation 33) and are independent of the pressure and source energy.

Strictly speaking, the definition of the W-value for the field case should include an allowance for energy gained to electrons in the electric field which then result in ionization. There is no way to include this energy transfer in the present case, so the values listed in Table 2 are based on the ion pair production divided by the energy input with the high-energy source electron alone (no field contribution). This is, then the same formulation (Eq. 65) as that of no field case, and we lable the result as the "effective" or "modified" W-value. Again these values fluctuate considerably, so the ranges observed in the last 10 time cycles are given, As would be expected from the neglect of the field contribution, the W-values in this table are in general smaller than that of no field case. As in the earlier calculation, no general trend can be observed, as so far as the dependence of the parameters (E_o, S_o, p) are concerned, and this is consistent with the earlier observations and the literature which indicate that the W-values are fairly insensitive to these parameters.

We have concluded so far that, the distribution functions for non-field case ($E_f = 0$) are more or less assume a Maxwellian distribution in the low-energy region for source rates below 10^{18}. However, when an electric field

is added, the distribution shifts to that found by Smit in the low-energy region. This is, in effect, the well-known Druyvesteyn distribution. It is significant that the addition of a source adds a tail to this distribution, but it does not drastically change the low-energy region. By intuition, it might be expected that Smit's distribution (with electric field or $E_f \neq 0$) would change back to a Maxwellian distribution as the electric field approaches zero. In order to display the transition region, the distribution functions for smaller electric field ($E_{f/p} = 1$) are plotted in Figure 26 together with the calculated distribution functions at $E_{f/p} = 10$ and $E_f = 0$. The high-energy tail of the distribution curve are not significantly affected by reducing the electric field E_f, but the distribution function in the low energy region starts to approach a Maxwellian distribution as expected.

D. Conclusion on Monte Carlo Results

Based on the Monte Carlo solutions we obtained so far, we can make the following comments.

1. For the normal range of source rate ($S \leq 10^{18}$), where the neglect of electron-electron interactions remains valid, the Maxwellian plus 1/E distribution is a good initial approximate distribution for the no electric field case. Likewise the Smit (or Druyvesteyn) plus 1/E distribution is a good approximate initial distribution to be used for the system with an electric field present.

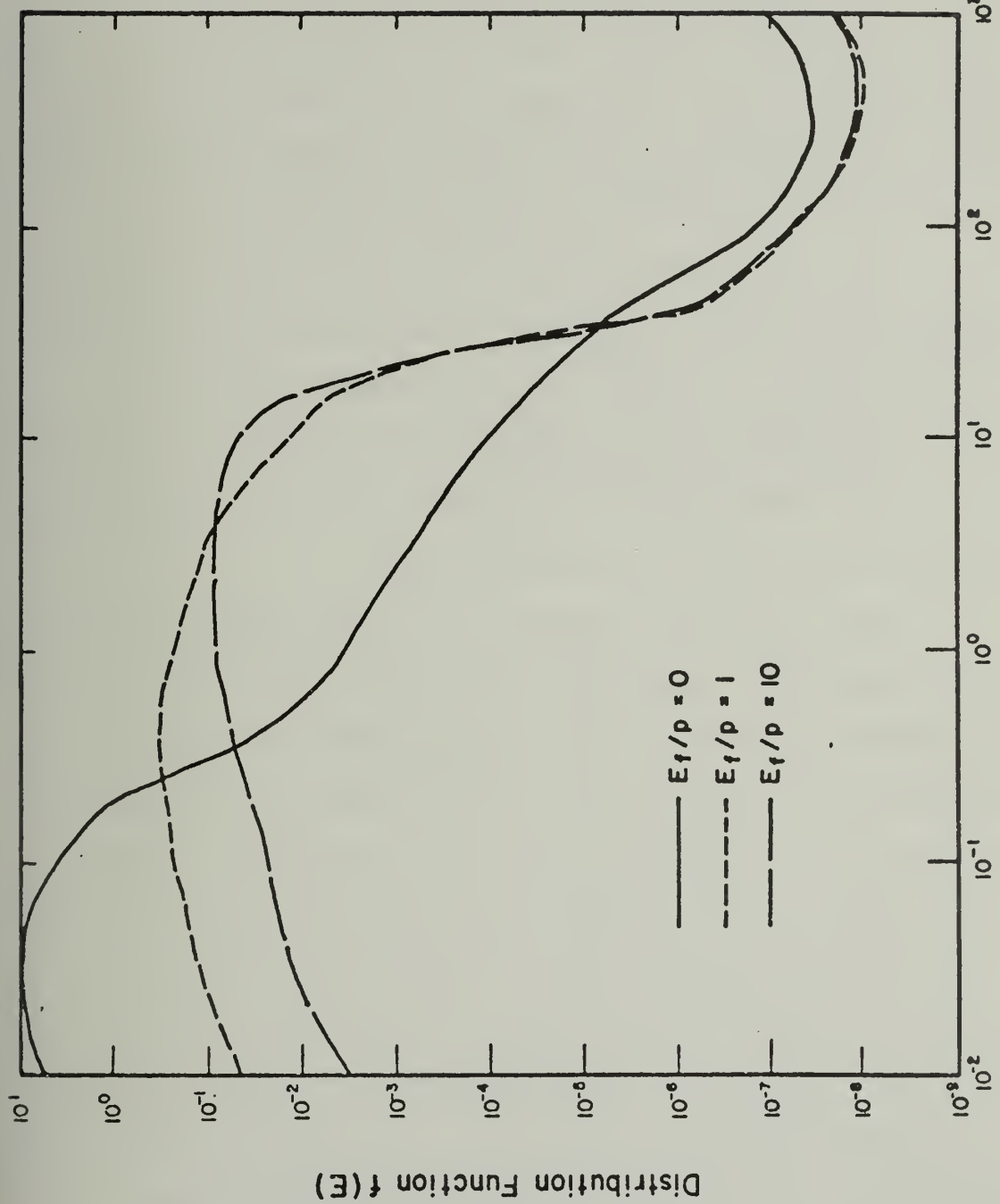


Figure 26. The electron energy distribution for He at p = 10 torr, $S_o = 10^{16}$ for $E_{f/p} = 0$, $E_{f/p} = 1$ and $E_{f/p} = 10$.

2. The dependence of the distribution functions (with or without electric field) upon the pressure and source rate only shows up in the high-energy region, where the distribution functions have higher tails for higher source rate, and have smaller values for higher pressures.

3. The range of variations observed in the W-value calculation reflects statistical fluctuations which limit the calculational accuracy of the absolute numerical W-values. Still the results demonstrate that the W-value is more or less independent or insensitive to the changes of pressure, source rate and source energy.

4. Due to a tight budget, the primary emphasis was on increasing the computation efficiency and reducing the computation time to a possible minimum. Thus most of the calculations were carried out with 2000 to 5000 actual particles and for any particular set of parameter values, and the results were generally obtained within 10 minutes of (IBM 360/75) computer time. Compared with hours of computer time and 5 to 10 times more particles used by others for the similar calculations (e.g., see References 3, 4, and 9) the gain in computation efficiency seems to be significant. Of course, a complete comparison is not possible since all of these calculations achieved different accuracies in the final results.

5. The present results also show close agreement with the analytic solutions of Lo and Miley (32,33) on the

following points:

a. The shape of high-energy portion of the distribution curves are in reasonable agreement as shown in Figure 9.

b. The high-energy part of the distribution function is not changed by the presence of an electric field for field values $E_{f/p} \leq 10$.

c. With an electric field, the low-energy part of the distribution function agrees with Smit's result; and this part is not affected appreciably by source rates $< 10^{18}$ particles/cm^3-sec.

CHAPTER VI

CONCLUSIONS

A. Prelude

The application of Monte Carlo techniques to solve particle transport problems is of fundamental interest in many fields of physics and engineering; especially when analytic and/or numerical solutions of the basic governing equations are too complex to be practical. Yet direct application of Monte Carlo techniques to simulate individual interactions is sometimes prohibitively costly because of the large amount of computational time required. Thus techniques for improving the efficiency are required. Various existing variance reduction techniques can be used, but they are problem dependent. Thus techniques that are efficient for one type of problem might not be as effective for other types of problems. Thus such techniques must be judiciously selected and modified for the particular problem under consideration. One basic underlying principle which applies to any Monte Carlo calculation is: Apply as much known information as one can (given in analytic and/or numerical form) to reduce the uncertainties of the problem. Whenever possible Monte Carlo experiments should be checked and replaced by exact theoretical analysis to reduce uncertainties.

The Monte Carlo experimentalist has to exercise ingenuity in distorting and modifying problems in the pursuit

of variance-reduction techniques. Although Monte Carlo methods are general devices, still a great deal of work depends upon the individual's originality to create special methods or numerical schemes to suit their needs. Unlike the physical experimentalist, the mathematical experimentalist using Monte Carlo Methods has the advantage that his experimental material consists of mathematical objects which can be distorted, controlled, and modified more easily.

The greatest successes of the Monte Carlo method have arisen where the basic mathematical problem itself consists of the investigation of some random processes. However, there are exceptions involving deterministic problem-solution of boundry value problems and partial differential equations. The solutions of these problems are closely connected with the characteristics of certain random diffusion type processes (or can be converted to such type of processes), therefore these problems are reduced to the modeling of such processes. Thus the model and the special techniques developed in present research are quite general in scope, and it should be possible to apply them to many classes of Monte Carlo calculations with a certain amount of modification.

B. Summary of Present Work

In this research study, we have devised a general mathematical model for the particle transport or diffusion

type plasma problems which have inherent nonlinear properties due to recombination. Many special variance reduction techniques are incorporated into the system. The model can be used for calculating both time-dependent and steady-state nonlinear transport problems provided that suitable methods exist to calculate, predict, and correct the important parameters which dominate the nonlinearities. A wide range of nonlinear problems can be formulated and handled in this way. The principle idea, the piecewise linearized predict-correct model, is a general, simple, and efficient approach for solving nonlinear problems. In principle, most nonlinear problems can be cast in terms of the basic ideas and algorithms of present work. This represents an extension of earlier works of Musha and Itoh (8), Thomas (9), and Fleck Jr. (11). As for the amount of computation time and efficiency involved, the present study has made significant improvements. Some of the improvements are a natural consequence of the large storage space available in modern computer systems. Additional improvements come from a few simple, but effective, special techniques incorporated into the present model. As described in Chapter II, these include:

1) The initial distribution - straightforward particle tracing procedures would require following every simulated particle from its birth (from source) with initial energy E_o at $t = t_o$ to the end of its life time history. This type of simulation would require hundreds

of cycle times to achieve a final steady state condition. Instead, we start with an apprixmately steady-state system by guessing an initial particle energy distribution. Then we simulate the system by tracing particles starting with energy corresponding to this input distribution. This is equivalent to skipping over the initial transient time cycles and greatly reduces the computation time and increases the calculation efficiency.

2) The application of the negatively-correlated variates (antithetic variates) technique greatly reduces statistical fluctuations with a minimum number of simulating particles (machine particles).

3) The introduction of a weighting scheme and an artificial game of chance (using weighted cross sections) contributed some reduction in calculation time and resolved some practical difficulties.

4) For the system with an applied electric frield, the exact formulation for a parabolic flight path was used to advance the particles in larger steps than would have been possible using the small-step linear approximation employed by Musha and Itoh (8) and also by Thomas (9). This improves the efficiency appreciably.

Throughout the entire calculation, one basic balance equation (Eq. 30) played a very important role. It merely states that at steady state, the source is balanced by losses.

By means of this equation, we predict the nonlinear parameter values and provide checks for convergence of the solution.

The need for large amounts of storage space for Monte Carlo calculations no longer creates serious problems or drawbacks on modern large computer systems, such as was the case as recent as seven or ten years ago. In addition, techniques exist for further reducing the storage requirement. In the present study, we suggest a technique to eliminate major storage requirements, and use only a small amount of storage as a temporary buffer storage (described later).

In other types of numerical solutions, e.g., in finite difference solutions of the diffusion equation, the step size Δt is restricted by stability requirements. However, in this present model, Δt is only restricted by the degree and amount of nonlinearities present in the system. This restriction is far less stringent.

C. Practical Limitations and the Cures

It was necessary to solve several difficulties in the present simulation study in order to provide practical solutions. We shall describe them item by item.

1) The electron energy distribution is the quantity of major interest. The difference between the magnitudes of its maximum and minimum non-zero values is of the order 10^9. This is due to high density in the low-energy region (thermal energy) and the relatively low density

in the high-energy region (near the source energy). It is unrealistic to hope to produce reasonable numbers of particles in the low-density (high-energy) region and at the same time have 10^9 times as many in the low-energy region. This problem is resolved by combining the following techniques:

a) Russian Roulette and splitting.

b) Weight factors which produce fractional particles.

c) Logarithmic energy intervals. The number of particles in each energy class interval ΔE_i is directly proportional to $f(E_i)\cdot\Delta E_i$ ($f(E_i)$: number density at E_i). By using logarithmic energy intervals, we have small intervals at low energy region and large intervals at high energy so that the product $f(E_i)\cdot\Delta E_i$ assumes a practical magnitude.

2) The total number of simulating particles (machine particles) N_T is limited by the storage requirement and the economy of the calculation (computing time is proportional to N_T). We have to set an upper limit (Nmax) on the total number of simulating particles in any time cycle. During each time cycle of duration Δt, N_s source particles are introduced into the system, and N_z secondary particles are produced (by ionization). At the same time N_{es} particles escape from the system, and N_{Ab} particles are lost due to recombination.

There are two conditions to be satisfied at all times:

a) $N_c + N_z + N_s \leq N_T \leq N_{max}$ (67a)

b) $N_z + N_s \simeq N_{es} + N_{AB}$ (67b)

where N_c: the number of census particles (background particles).

Condition a) insures that total number of particles in the system is always under the limit (Nmax). Condition b) indicates that a particle balance should be satisfied at steady state.

In the program, there are two equivalent problems to be considered. One is the balance of the machine particles [corresponding to condition (a)], and the other is the balance of simulated particles [weighted particles, corresponding to condition (b)]. Both conditions must be satisfied simultaneously. Condition (a) allows a certain amount of leeway since the number of particles that survive the integration cycle (time cycle) and hence require storage will be less than $N_c + N_z + N_s$. Here N_s is chosen to be an input number, the weights of these particles are determined by the source rate. If condition (a) can not be met, N_s is taken to be

$$N_s = N_{max} - N_c - N_z - JZ - 1 \quad (68)$$

where JZ is the number of spatial zones. It has been shown (12) that Equation 68 insures the stabilization of census population without overly reducing the number of source particles.

The proper selection of the energy dividing line (EDl) for Russian Roulette and splitting can insure the satisfaction of condition (b). Also as mentioned in earlier chapters, the balance factor (BF) is used to speed up convergence and force condition (b) to be satisfied sooner.

3) In any Monte Carlo calculation, finite samples are used to estimate or simulate the behavior of a large parent population. This is the main source of statistical fluctuations (variance or uncertainty). In the present simulating system, less than 5000 particles were used to simulate approximately 10^{14} physical particles. This creates the problem of matching the values of input and estimated output quantities. Due to the huge scaling factor ($10^{14}/5000$), a small amount of statistical fluctuation or estimation error in the estimated value will be amplified about 10^{11} times. To avoid this, we use the estimated (or equivalent) input quantities which carry the same order of magnitude of statistical fluctuation and weight.

4) There are several reasons that make the logarithmic energy scale the logical choice for the group intervals in the energy axis of phase space. These include:

   a) the wide energy span (0 to 1500 eV)

   b) the relatively high number density at low energies combined with a low rate and small amount of energy

exchange due to collision processes. In the high-energy region, the situation is just the opposite.

c) to produce reasonable number of particles in each energy interval [for the reason mentioned in the first section (II-B-1)]. The size and number of intervals are mainly dictated by the range of data (energy range in this case) and number of observations available. Excessive fragmentation of the data may produce many intervals with few occupants. On the other hand, insufficient divisions may obscure important dispersions. Thus an optimum number of intervals will be a compromise between these extremes.

D. Future Extensions

The Monte Carlo methods are applicable to the most widely diverse branches of computational mathematics including particle physics (neutron transport for instance), operations research problems such as the investigation of servicing processes, modelling the processes of information transmission in communication theory, the evaluation of definite integrals, the solution of partial differential equations (e.g. boundry-value problems); the solution of systems of linear equations - inversion of matrices, and many other applications. Problems handled by such methods are in general of two types, the probabilistic and the deterministic, according to whether or not they are directly concerned with the behavior and outcome of random processes.

Their basis lies in simulating statistical experiments by means of computational techniques. Based on the underlying principles described earlier, various variance reduction techniques can be applied. The present work serves as an example and guide for using the important new techniques such as correlated sampling.

1) The code developed can readily be used to calculate electron energy distribution functions for other gaseous media by merely changing the cross sections input. The model can also be modified to include the electron-electron and electron-ion interactions although this adds more nonlinearities into the system. This would allow calculation for higher source rates and cases where the fractional ionization is large.

2) As for the complex transport problems encountered in areas such as plasmas physics and astrophysics, the model and techniques can readily be extended to the problems with more complex geometry and/or boundry conditions, with inhomogeneous media and multi-dimensions. Also many kinds of nonlinear features can be studied in a realistic fashion.

3) More elaborate error checking and correction procedure (based on the known physical phenomena or theoretical formulations) such as the correction matrix used by Berger (9) should be developed to treat the combined effect of statistical fluctuations and other types of

uncertainties. This is essential for generating good results for Monte Carlo calculation.

4) More elaborate algorithms or techniques for playing the artificial games of chance by means of weighted cross sections would be a good direction for future research. This must be based on the investigator's intuition and experience, but still it is a promising approach for increasing the efficiency.

5) The present model and techniques can be also implemented on smaller computer systems such as PDP-11 or other similar systems where large amount of fast storage space are not available. The following techniques could be used to process the calculation without storing all the particle data (namely E_i, u_i, z_i, Wt_i Ψ_i). At the beginning of each time cycle, we generate a small number (some reasonable amount, $\simeq$ 100 for instance) of particles. The corresponding particle data can be generated from the initial input distribution or from last time cycle. After these particles have been processed, only the accumulated information is stored. A new group of particles come into the system by generating a new set of data, based on the same distributions, which are stored in the same temporary storage space. The previous particle data is destroyed after they have been processed. The same process is repeated until all the necessary prespecified number of particles have been

processed, and the new distributions are obtained. This eliminates the necessity of storing all the particle data at each time cycle, and this eliminates the large arrays that demand the major amounts of storage space. Due to the random nature of the processing algorithms, and the Markovian behavior of the time cycle process (these time cycle processes are a kind of Markov process), this storage saving algorithm can accomplish the desired results.

E. Concluding Remarks

In developing any Monte Carlo models and performing calculations, as mentioned in Chapter V the systematic errors and outright blunders must be detected and removed by testing and comparing with known results.

The various variance reduction techniques are used to increase the relative computation efficiency, reduce inherent random errors or statistical fluctuations. For better calculational results, more samples are favorable even though not economic. In any Monte Carlo calculation there exists a minimum number of samples below which the results or statistics are no longer valid and dependable regardless of the variance reduction schemes employed. In the other words, variance reduction techniques help to reduce statistical fluctuations, but they can not be used to remove all the fluctuations caused by small samples.

The minimum sample size, is, of course, problem dependent. There are no definite rules or formula for it, thus a cut and try method is necessary until the calculated variance is acceptable.

Monte Carlo calculations are perhaps best in the preliminary stages where they help to give a general idea of the situation and give hints or feelings for trends. If more accurate results are necessary, Monte Carlo calculations may not always be practical good method. In any case, the Monte Carlo method is an important tool in the inferential analysis of the mathematical-physics problems, but it should be viewed as supplementing, rather than replacing, analytic and other numerical methods.

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APPENDIX

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FORTRAN IV G LEVEL 18                MAIN          DATE = 72126        05/31/02

      C MASTER PROGRAM OF MONTE CARLO SIMULATION OF NONLINEAR ALPHA PLASMAS (ALPHA PAR
      C TICLES INDUCED PLASMA ELECTRON ENERGY DISTRIBUTION STUDY
      C DEFINITIONS AND TERMINOLOGY
      C D: DIAMETER OF THE CYLINDER THE LENGTH OF THE FINITE REGION
      C EO:INITIAL ENERGY OF THE SOURCE PARTICLES SO(NS): SOURCE RATE
      C JZ:TOTAL NUMBER OF ZONES   JE: TOTAL NUMBER OF ENERGY RANGES
      C IAS: ARRAY FOR STORING THE INDEX OF ABSORPED PARTICLES NAS: THE NO. OF THEM
      C DB: DISTANCE TO BOUNDRY  DCOL: DISTANCE TO COLLISION  DCEN: DISTANCE TO CENSUS
      C DZ: ZONE INTERVAL
      C ARRAYS E, Z, U  STORING ENERGY, DISTANCE, AND DIRECTION OF PARTICLES
      C NTP: TOTAL NUMBER OF PARTICLES TO BE PROCESSED  EACH CYCLE
      C NT: TOTAL NUMBER OF TIME CYCLES
      C NS: NUMBER OF SOURCE PARTICLES PER UNIT TIME*DISTANCE  OR SOURCE RATE
      C NIZN: NUMBER OF IONIZATION PROCESS OCCURRED EACH TIME CYCLE
0001          REAL    NE(55), NEZ( 55,10),EZ(11),DX(3),EE(55),  CEZ(11),EKZ(55
     1,10) ,FID(60),NREZ(11),EZI(11),NTPW
0002          DIMENSION  ENE(55), ENREZ(11), NRZI(11),CNE(55), CNREZ(11),TNE(55)
0003          COMMON D, E(5100),Z(5100), U(5100) ,IAS(500),IRR(850),NRR,IES(600)
     X,WT(5100),SWF
0004          COMMON /AREA1/ NIZN, NOZN, NAS, DIZN(500),NSE, NMET, NEXC, ETAS  ,
     XWNMET, WNEXC, WNIZN, ELS,WNAS ,WNSE
0005          COMMON /AREA2/ C1,MUO,EI,EIS,SF,ANEAM,PDPO,PI,EO,NION,JE,JZ,NASW1,
     1NSEW ,AKT, AIKT ,AM1 ,AMC1,ED1,PDMUC, PD26,K1, K2, K3, WN2,ED2,ED3
0006          COMMON /AREA3/ XSEL,XELC,XRCB,XMET,XEXC,XION,XTOL,KELC
0007          COMMON /AREA4/  CONST,DEL2, ELT,IE, DII, DI2, DI3 ,DELI
0008          COMMON /A5/ EG(55), EDE(55), EBD(55)
0009          COMMON /A6/ ESE(50) , NUP ,NDNR,NDN, WSE(50)
0010          REAL  MUO, NION,ND
      C STATEMENT FUNCTION FOR EVALUATING  MAXWELLIAN AND RELATED FCNS
0011          FM1(E,FNEM)=EXP(-E*AIKT)*SQRT(E)*FNEM
0012          DATA  TMS,NT,DTDT,ETDT,NIN,NIZNT,NAST/0.0,1,0.0,0.0,0,0,0/
0013          DATA W5VLE,CN5IZ,CN5S,CNES,CNAS,CNMET,CNEXC,CESAVG,CEASG/9*0.0/
0014          DATA CNE/ 55*0.0/, CEZ/11*0.0/, CNREZ/11*0.0/,TNE/55*0./,EKZ/550*0
     1.0/,D5AVS/0.0/
0015          DATA NEZ/ 550*0./,NE/55*0./,EZ/11*0./,NREZ/11*0./,EE/55*0.0/
0016          READ(5,1) NTAPE
0017          READ(5,151) K1, K2, NTC, NTP,NTW,NPM, KELC ,JZ, IM,NCUM, NDPN,NTVP
     X, MC ,IUSN, NUST, NBF
0018          READ(5,152) ED1 ,ND , EO,ANSW, D, EDP, PDPO, SR
0019          READ(5,153) FID
0020        1 FORMAT ( I10)
0021      151 FORMAT( 16I5)
0022      152 FORMAT( BF10.4)
0023      153 FORMAT( BE10.3)
0024          DELE=1.0
0025          DELI=1.0/DELE
0026          DEL2=2.0
0027          AKT=0.05
0028          AIKT= 1.0/AKT
0029          PI=3.141593
0030          EMASSI=1.60203E+16/9.108
0031          K3=K1*K2
0032          WN2=1.0/K2
```

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FORTRAN IV G LEVEL  18                  MAIN                    DATE = 72126          05/31/02

0033                CJD=0.0
0034                E1=24.46
0035                EF=EDP*PDPO
0036                EIS=21.4
0037                C1=2.0*0.000549/4.003873
0038                ETV= SQRT(2.0*1.60203/9.108)*1.0E+08
0039                VTE= 1.0/(ETV*ETV)
0040                CALL  UNDERZ('OFF')
0041                PD26=PDPO*26.0
0042                MUO=(1.0E-09)/ETV
0043                CMUO=1.0E-09
0044                CMUPDP=CMUO*PDPO
0045                IF (PDPO.GT.10.0)  CMUPDP=CMUO*10.0
0046                PDMUO=CMUPDP/ETV
0047                ELS=1.0
0048                NUP=0
0049                NDN=0
0050                NDNR=0
0051                INO=0
0052                NRR=0
0053                NAS=0
0054                NES=0
0055                NSE=0
0056                NOZN=0
0057                NIZN=0
0058                NIN=0
0059                LK=0
0060                INIV=999999
0061                NMET=0
0062                NEXC=0
0063                ETAS=0.0
0064                ETEP=0.0
0065                NTP5=0
0066                NW=0
0067                N5TP=0
0068                NCOL=0
0069                WNMET=0.0
0070                WNIZN=0.0
0071                WNEXC=0.0
0072                WNAS=0.0
0073                WNES=0.0
0074                WNSE=0.0
0075                CLOSS=0.0
0076                CSF2=0.0
0077                CNIO2=0.0
0078                CSF1=0.0
0079                CETAS=0.0
0080                CETEP=0.0
0081                DTAVS=0.0
0082                JE=48
0083                IE=JE
0084                DEN=3.54E+16*PDPO
0085                DETZ=D/JZ
```

```
FORTRAN IV G LEVEL  18                  MAIN                    DATE = 72126          05/31/02

0086              DZIV= 1.0/DETZ
0087              CONST=1.0/ALOG(2.0)
0088              ED2=0.447513
0089              ED3=19.8
0090              PM=ED2*AIKT
0091              AM1=2.0*AIKT/SQRT(PI*AKT)
0092              CALL   RN3INZ(9945632111)
0093              SO=PDPO*SR*1.0E+16
0094              SF=1.0
0095              AITG=  CMUPDP /(AKT*PI)
0096              DE1=0.016
0097              DE2=0.355
0098              DE3=0.3
0099              DI1=1./0.016
0100              DI2=1./DE2
0101              DI3=1./DE3
0102              AMC1= SQRT(2.0*2.7183*AIKT)*ED2
0103              DO  11  I=6, 36
0104              EBL =(I-5)*DE2 -4.0
0105              EMV= EBL -0.1685
0106              EBD(I)= 2.0**EBL
0107              EG(I-1)= 2.0**EMV
0108           11 EDE(I)=EBD(I)*(2.0**DE2 -1.0)
0109              JE1=JE+1
0110              DO  12  I=37, JE1
0111              EBL= 7.005 +(I-36)*DE3
0112              EMV= EBL - 0.1405
0113              EBD(I)= 2.0**EBL
0114              EG(I-1)= 2.0**EMV
0115           12 EDE(I)= EBD(I)*(2.0**DE3 -1.0)
0116              DO  10  I=1, 5
0117              EDE(I)= 0.016
0118              EG(I)= EDE(I)*I -0.008
0119           10 EBD(I)= EDE(I)*(I-1)
0120              EDE(36)=29.69
0121              EG(48)= 1737.482
0122              IF  (NTAPE.NE.1)  GO  TO  2
0123              READ(10)  EAVG, DAVG, TME, NTW, NT, NTP, NION, DDEG, NSW,SWF, E,U
0124              READ(10) Z, WT, ANIOS,SF3
0125              NS=NSW*K2
0126              WGHT=1.0
0127              REWIND  10
0128              NT=NT+1
0129            2 CONTINUE
0130              IF (NTAPE.NE.2)  GO  TO  5
0131              READ(9 )  EAVG, DAVG, TME, NTW, NT, NTP, NION, DDEG, NSW,SWF, E, U
0132              READ(9 ) Z, WT, ANIOS,SF3
0133              NS=NSW*K2
0134              WGHT=1.0
0135              REWIND  9
0136              NT=NT+1
0137            5 CONTINUE
0138              IF  (NTAPE.NE.0)  GO  TO  122
```

```
FORTRAN IV G LEVEL 18                MAIN                DATE = 72126          09/31/02

0139              NION= SQRT(SO*10/AITG)
0140               ANEAM=NION*0.33333/DEN
0141              CALL  SORCE2(NTP, EAVG, NTW, PM, FID)
0142              AL=ALDA(EAVG)
0143              DAVG=AL
0144              DDEG=DAVG*ND/SQRT(EAVG)
0145               SF2=1.0
0146              IF  (NION.NE.0)  SF2=NTW/NION
0147              SN=SO*AL*ND*SF2/(ETV*SQRT(EAVG))
0148              NSW=ANSW +0.5
0149              IF (SN.GT.ANSW)  NSW=SN +0.5
0150              NS=NSW*K2
0151              SWF=NSW/SN
0152              SF=SWF
0153              SF1=SF2
0154              SF3=SF2
0155              CALL  SOURCE(NS,NTP)
0156              TME=0.0
0157              ANIOS=NION
0158              WGHT=1.0
0159            '122 CONTINUE
                C  GENERATE SOURCE PARTICLES TO INITIALIZE THE PROGRAM
0160              ANEAM=NION*0.33333/DEN
0161              WRITE(6,70)
0162             70 FORMAT('1','PROGRAM INITIALIZATION AND THE INITIAL PARAMETERS',//)
0163               WRITE(6,71) AITG, NION, NTP, AL,EAVG
0164             71 FORMAT(' ', 'AITG =',E14.6, 3X,'NION =',E14.6,3X,'NTP =',I12,3X,
                   1'DCEN(EO) =', F14.6,3X, 'EAVG= ',F14.4,/)
0165             72 FORMAT(' ',8X,'DCOL',13X,'DCEN',13X,'ENERGY',11X,'Z',14X,'U', 10X,
                   X'WEIGHT',/)
0166             75 FORMAT(' ',F14.6,3X, F14.6, 3X, F14.5,3X, F12.4,3X,F12.4,3X,E13.4)
0167              WRITE(6,72)
0168              RIP=RAN3Z(0)
0169              I=1
                C WITHIN THE OUTER I LOOP THE I TH PARTICLE HISTORY
                C  GEOMETRIC ROUTINE ENTERING HERE
0170           7777 IF ((E(I).LE.0.0).OR.(E(I).GT.EO*1.5))  GO  TO  9008
0171              TCEN=DDEG/ETV
0172           7778 IF ((NIZN.GT.0).AND.(I.GT.NTP))  TCEN= DIZN(NOZN+1)
0173              U(I)=U(I)*IUSN
0174              LFG2=0
0175              ETAG1=1.0
0176              IF (E(I).GT.ED1) ETAG1=-1.0
0177              SQE= SQRT(E(I))
0178              DVA=EF*TCEN*EMASSI*0.5
0179              VZA=SQE*ETV*U(I) + DVA
0180              VYS=E(I)*ETV*(1.0-U(I)*U(I))*ETV
0181              DCEN= SQRT(VZA**2+VYS)*TCEN
0182              NFLG=0
0183            900 IF (E(I).LE.0.0)  GO  TO  9008
0184              IF  (NFLG .EQ.0)  GO  TO  809
0185              SQE= SQRT(E(I))
0186              DVA=EF*TCEN*EMASSI*0.5
```

```
FORTRAN IV G LEVEL  18                  MAIN                DATE = 72126          05/31/02

0187                VZA=SQE*ETV*U(I) + DVA
0188              809 DZ=VZA*TCEN
0189                ENEW= E(I) + EF*DZ
0190                IF (ENEW.LE.0.0)  GO  TO  9008
0191                SQEP=SQRT(ENEW)
0192                UNEW= SQE*U(I)/SQEP +DVA*2./(SQEP*ETV)
0193                AL1=ALOA(E(I))
0194                AL2=ALOA(ENEW)
0195                ALI=1.0/AL1 + 1.0/AL2
0196                ALO=2.00/ALI
0197                RI=RAN3Z(0)
0198                ALR=ABS(ALOG(RI))
0199                OCOL= ALR*ALO
0200                IF (NFLG.EQ.1)  GO  TO  901
0201                IF(MOD(I,IM).EQ.0)  WRITE(6,75)    DCOL,OCEN,E(I),Z(I),U(I),WT(I)
0202                OCOL2=ABS(ALOG(1.-RI))*ALO
0203                OTOT=OTOT +OCOL+OCOL2
0204                ETOT=ETOT+E(I)
0205                IF (NOPN.LT.2)  GO  TO  901
0206                TCEN2=TCEN
0207                OCEN2=OCEN
0208                EIO=E(I)
0209                UIO= U(I)*IUSN
0210                ZIO=Z(I)
0211                ENWO=ENEW
0212                UNWO=UNEW
0213                OZO=DZ
0214              901 NFLG=1
0215              902 IF  (OCEN.LT.OCOL)  GO  TO  905
0216                TCEN=TCEN - OCOL*TCEN/OCEN
0217                 OZC=OZ*OCOL/OCEN
0218                E(I)=E(I) + EF*OZC
0219                Z(I)=Z(I) +DZC
0220                OCEN= OCEN -OCOL
0221                NCOL=NCOL+1
0222                IF (MOD(NCOL,MC).EQ.0) RIP=RAN3Z(0)
0223                IF (MOD(NCOL,MC).NE.0) RIP=1.0-RIP
0224                CALL  COLPRO(I, TCEN, NTP, RIP, NUST, &9008, &9045)
0225                IF((E(I).LE.0.0).AND.(LFG2.EQ.1))  GO  TO  9008
0226                GO  TO  900
0227              905 E(I)=ENEW
0228                U(I)= UNEW
0229                Z(I)= Z(I) + DZ
0230                IF ((Z(I).LE.0.0).OR.(Z(I).GT. D ))   GO  TO  9008
0231                J=INT(Z(I)*DZIV)+1
0232                IF (J.GT.JZ)   J=JZ
0233                K= INDEXE(E(I))
0234                IF (K.GT.JE) K=JE
0235                IF (K3.EQ.1)  GO  TO  904
0236                ETAG2=1.0
0237                IF (E(I).GT.ED1)  ETAG2=-1.0
0238                IF ((ETAG1*ETAG2).GT.0.0)  GO  TO  904
0239                IF (ETAG2.GT.0.0)  GO  TO  903
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0240            NUP=NUP+1
0241            ESE(NUP)=E(I)
0242            WT(I)=WT(I)/K3
0243            WSE(NUP)=WT(I)
0244            GO  TO  904
0245          903 IF((LFG2.EQ.1).OR.(NDPN.LT.2))  NDNR=NDNR+1
0246            IF((LFG2.EQ.1).OR.(NDPN.LT.2))  IRR(NDNR)=I
0247            NDN=NDN+1
0248            IF (MOD(NDN,K3).NE.0)  GO  TO  9045
0249            WT(I)=WT(I)*K3
0250          904 NEZ(K,J)= NEZ(K,J) + WT(I)
0251            EKZ(K,J)=EKZ(K,J)+E(I)*WT(I)
0252         9045 IF((LFG2.EQ.1).OR.(NDPN.LT.2))  GO  TO  9009
0253            LFG2=1
0254            E(I)=EIO
0255            U(I)=UIO
0256            Z(I)=ZIO
0257            TCEN=TCEN2
0258            DCEN=DCEN2
0259            DCOL=DCOL2
0260            ENEW=ENWO
0261            UNEW=UNWO
0262            DZ=DZO
0263            IF (IUSN.LT.0)  GO  TO  900
0264            GO  TO  902
0265         9008 NES=NES+1
0266            IF (E(I).LT.ED1) WT(I)=WT(I)/K3
0267            IF (WT(I).GT.1)  WT(I)=1.0
0268            WNES=WNES +WT(I)
0269            IES(NES)=I
0270            IF  (E(I).GT.0.0)  ETEP=ETEP+E(I)*WT(I)
0271         9009 I= I+1
0272            LFG2=0
0273            IF (I.LE.NTP)  GO  TO  7777
0274            IF ((I.GT.NTP).AND.(NIZN.GT.0))  NOZN= NOZN-1
0275            IF (NOZN.LT.0)  NIN=1
0276            IF ((NIZN.GT.0) .AND.(NIN.EQ.0))  GO  TO  7778
0277            NIZW=WNIZN +0.5
0278            NWS=WNES +0.5
0279            NASW=WNAS  +0.5
0280            WNAS=WNAS/KELC
0281            WNSE=WNSE/KELC
0282            NSEW=WNSE +0.5
0283            DO  191  M=1,JE
0284            DO  191  N=1,JZ
0285            EE(M)=EE(M) + EKZ(M,N)
0286          191 NE(M)= NE(M) + NEZ(M,N)
0287            IF ((K3.EQ.1).OR.(NUP.EQ.0))  GO  TO  24
0288             N3=K3/JZ
0289            IF  (N3.LT.1)  M3=1
0290            NK3=K3-1
0291            IF (NK3.LT.JZ) IZ=NK3
0292             IF (N3.GE.1)  M3=N3
```

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0293                DO  23  N=1,NUP
0294                K=INOEXE(ESE(N))
0295                EE(K)=EE(K) + (K3-1)*ESE(N)*WSE(N)
0296                NE(K)=NE(K) +(K3-1)*WSE(N)
0297             22 IF (NK3.GE.JZ)  IZ=JZ
0298                DO  21  L=1,IZ
0299                NREZ(L)=NREZ(L) + M3*WSE(N)
0300             21 EZ(L)=EZ(L) + ESE(N)*M3*WSE(N)
0301                NK3=NK3 -JZ*M3
0302                IF (NK3.LT.JZ)  IZ=NK3
0303                M3=1
0304                IF (NK3.GT.0)  GO  TO  22
0305             23 CONTINUE
0306             24 CONTINUE
0307                DO  192  M=1, JZ
0308                DO  1915  N=1,JE
0309                NREZ(M)=NREZ(M) + NEZ(N,M)
0310           1915 EZ(M)=EZ(M) +EKZ(N,M)
0311            192 CONTINUE
0312                NTPN=NTP+NIZN-NES-NAS
0313                NTPW=0
0314                ETOL=0.0
0315                DO  14  M=1,JE
0316                ETOL= ETOL +EE(M)
0317             14 NTPW=NTPW +NE(M)
0318                EWTOL=ETOL
0319                NTPT=NTPN
0320                DAVGO= OAVG*ND
0321                DAVS=(OAVGO*1000.)**NTVP
0322                D5AVS=D5AVS+ DAVS
0323                OTAVS=OTAVS +OAVS
0324                OI5G=1.0/D5AVS
0325                ANTPO = 1.0/NTPW
0326                N5TP= N5TP + NTPW +0.5
0327                NTP5=NTP5+ NTPN*DAVS
0328                NTPO=NTP
0329                EWAVG=EWTOL*ANTPO
0330                NSO=NS
0331                NSWO=NSO*WN2 +0.5
0332                NTP=NTP+NIZN
0333                NTPP=NTP
0334                OAVG=DTOT*0.5/NTP
0335                EAVG= ETOT/NTP
0336                OEG=DOEG/ETV
0337                TME=TME+DEG
0338                TMS=TMS+DEG
          C IF SOURCE PARTICLES SO(NS)< NES THEN ELIMINATE AS MANY RESIDUE PARTICLES AT TH
0339                NTPS=NTPW+ NWS +NASW
0340                NTW=NTPW +.5
0341                OCENI= ALOA( EAVG)
0342                OOEG=DAVG*NO/SQRT( EAVG)
0343                BF=1.0
0344                IF  ((WNES+WNAS).GT.0.0)  BF=(WNIZN+SN)/(WNES+WNAS)
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0345              SF2=1.0
0346              IF (ANIOS.NE.0)  SF2=NTPS/ANIOS
0347              ESAVG=0.0
0348              IF(WNES.NE.0.0)  ESAVG= ETEP/WNES
0349              EASAVG=0.0
0350              IF (WNAS.NE.0)  EASAVG=ETAS/WNAS
0351              SWFO=SWF
0352              CN5S=CN5S+ SN*DAYS*WGHT
0353              CSF1= CSF1 +(ETEP+ETAS+40.*WNIZN)/TMS
0354              SF1=CSF1*DI5G/(SO*EO)
0355              CSF2= CSF2 + SF2*DAYS
0356              IF ((MOD(NT,5).EQ.0).AND.(NT.NE.0))  SF3=CSF2*DI5G
0357              WGHT=SF1/SF3
0358              SN=SO*DDEG*SF3/ETV
0359              IF (NTP.GT.4920)  ANSW=2
0360              NSW=ANSW +0.5
0361              IF (SN.GT.ANSW)  NSW=SN +0.5
0362              SWF=NSW/SN
0363              NS=NSW*K2
0364              SF=SWF
0365              NMEW=WNMET +0.5
0366              NEXW=WNEXC +0.5
0367              W5VLE=W5VLE+ WVALUE*DAYS
0368              CETEP=CETEP + ETEP*DAYS
0369              CETAS=CETAS +ETAS*DAYS
0370              CN5IZ=CN5IZ+WNIZN*DAYS
0371              CNES=CNES+WNES*DAYS
0372              CNAS=CNAS+WNAS*DAYS
0373              CNMET=CNMET+WNMET*DAYS
0374              CNEXC=CNEXC+WNEXC*DAYS
0375              CESAVG=CESAVG+ ESAVG*DAYS
0376              CEASG=CEASG+EASAVG*DAYS
0377              CLOSS= CLOSS+(WNIZN-WNES)*DAYS/(TMS*SF3)
0378              WVLE1=W5VLE*DI5G
0379              NSAVG=CN5S*DI5G +0.5
0380              NIZAVG=CN5IZ*DI5G +0.5
0381              ANIZVG=CN5IZ*DI5G
0382              ANSVG=CN5S*DI5G
0383              AETEP=CETEP/DTAVS
0384              AETAS=CETAS/DTAVS
0385              IF (ANIZVG.NE.0)  WVLE2=(EO*ANSVG-AETEP-AETAS)/ANIZVG
0386              ALOSS=CLOSS*DI5G
0387              ANES=CNES/DTAVS
0388              ANAS=CNAS/DTAVS
0389              AESAVG=CESAVG*DI5G
0390              AEASG=CEASG*DI5G
0391              ANMET=CNMET*DI5G
0392              ANEXC=CNEXC*DI5G
0393              ANS=ANES+ ANAS -ANIZVG
0394              IF (ANS.LE.0.0)  ANS=NSW/SWF
0395              IF (WNIZN .NE.0.0)  WVALUE= (SN*EO*WGHT-ETEP- ETAS)/WNIZN
0396              IF (ANIZVG.NE.0)  WVC=(ANS*EO-AETEP-AETAS)/ANIZVG
0397              IF (NS.GE.1)  TMS=0.0
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0398                NET=NES+NAS
0399                CALL  SOURCE(NS,NTP)
0400                 IF (NET.GT.0)  CALL  FILHOL(NTP,NES, NAS)
0401              90 NIZNT= NIZNT +NIZW
0402                IF  (NUP .GT.0)  CALL  SEPROC(NTP, K3)
0403                IF (NONR.GT.0)  CALL  RRPROC(NTP,K3)
0404                NAST= NAST +NWS
                  C  INTROOUCE THE SOURCE PARTICLES FOR THE NEXT CYCLE
                  C EVERY FIFTH CYCLE RENORMALIZE NION AND OUTPUT QUANTITIES ARE PRINTED
                  C RENORMALIZATION PROCESS OF NION
0405                AN5TP= 1.0/N5TP
0406                ANTP5=D5AVS/NTP5
0407                N5TPN=N5TP
0408                OO  16  M=1,JZ
0409                CNREZ(M)= CNREZ(M) + NREZ(M)*OAVS
0410              16 CEZ(M)= CEZ(M) + EZ(M)*OAVS
0411                OO  18  M=1,JZ
0412                FNREZ(M)=NREZ(M)*ANTPO
0413              18 EZ(M)= EZ(M)/ NREZ(M)
0414                SUMNE=0.0
0415                OO   193  M=1,JE
0416                SUMNE= SUMNE + NE(M)
0417                TNE(M)= TNE(M) + NE(M)/EOE(M)
0418             193 FNE(M)=NE(M)*ANTPO/EDE(M)
0419                EAV3=0.
0420                OO  1755  M=1, JE
0421                EAV3= EG(M)*FNE(M)*EDE(M) +EAV3
0422             1755 CNE(M)= TNE(M)*AN5TP
0423                CNION=CMUPOP*2.0*AIKT/SQRT(AKT*PI)
0424                ANION=0.0
0425                ANIO2=0.0
0426                OO  20  M=1,JE
0427                ANIO2= ANIO2 + FM1(EG(M),CNE(M))*EDE(M)
0428                ANION= ANION + FM1(EG(M),FNE(M))*EDE(M)
0429              20 CONTINUE
0430                ONION=ANION*CNION
0431                ONIO2=ANIO2*CNION
0432                CJO=ALOSS
0433                IF (ALOSS.LT.0.0)  CJO=0.0
0434                IF (ABS(CJO).GT.110.*SO)  CJO=110.*SO
0435                TNION=ABS(SO+CJO)/ONION
0436                TNIO2=ABS(SO+CJO)/ONIO2
0437                TNIO2=SQRT(TNIO2)
0438                TNION=SQRT(TNION)
0439                CNIO2=CNIO2 + TNIO2*OAVS
0440                ANIOS=CNIO2*015G
0441                WF=1.0
0442                IF (ANES+ANAS.NE.0.)  WF=(ANIZVG+ANSVG)/(ANES+ANAS)
0443                IF  (MOO(NT,NPM).NE.0)  GO  TO  1790
0444                NION=ANIOS
0445                IF ((WF.GT.0.005).AND.(WF.LT. 200.)) NION=ANIOS*WF**NBF
0446             1790 CONTINUE
0447                OAVT=OAVG*NO
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0448                  ALPHA=WNIZN/(NTPW*DAVT)
0449                  ANEAM=NION*0.33333/DEN
0450               1785 FORMAT('0','ANION=',E13.4,3X,'ONION=',E13.4,3X,'TNION=',E13.4,3X,
                     X'ALPHA=',F12.5,4X,'LEAK=',E13.4,/)
0451                  WRITE(6,1785)  ANION, ONIO2, TNIO2, ALPHA, ALOSS
0452                  WRITE(6,171)  EO, PDPO, D, DETZ, DEG, NDPN
0453               171 FORMAT('1','GAS: HE',2X,'SOURCE ENERGY:',F5.0,3X,'PRESSURE:',F4.0,
                     X 'TORR',3X,'SLAB THICKNESS:',F4.1,' CM',' DX:',F4.1,' CM',4X,'DELT
                     X=',E12.5,3X,'#PROC=',I2,/ )
0454                  WRITE(6,180) NT, TME, NS,NSW
0455               180 FORMAT(' ','NUMBER OF TIME CYCLES=',I6,3X,'TIME =', E12.5,' SEC',
                     13X, 'GENERATED SOURCE PART =', I5,3X, 'WGTED # OF SOURCE PART.=',
                     1I5 )
0456                  WRITE(6,1805) DAVT, DCEN1,EAVG,EWAVG, EAV3
0457               1805 FORMAT(' ','DAVG =',F12.5,3X, 'DCEN =',F12.5,3X,'OVERALL EAVG=',
                     1F10.5,3X,' WGTED EAVG=',F10.5,3X, 'EAVG CHECK=',F10.5,/)
0458                  WRITE(6,181)
0459               181 FORMAT(' ', 1X,'NUMBER DISTRIBUTION',2X, 'FLUX DENSITY',4X,'AVERAGE
                     1E ENERGY',3X,'CUMULATED # DISTR',3X,'ENERGY INTERVAL',2X,'CUM FLUX
                     XDEN',4X,'#DEN-DEVIATION',/)
0460                  CESUM=0.0
0461                  DO  281  M=1, JE
0462                  CESUM=CESUM + CNE(M)*EDE(M)
0463                  IF (NE(M).GT.0)  DEAVG=EG(M)-EE(M)/NE(M)
0464                  IF (NE(M).LE.0)  DEAVG=0.0
0465                   IF (NE(M).EQ.0)  DNAVG=0.
0466                  FNDV=CNE(M)-FNE(M)
0467                   VFE=SQRT(EG(M))*ETV
0468                  FLX1=FNE(M)*VFE
0469                  FLX2=CNE(M)*VFE
0470                  IF (NE(M).EQ.0)  GO  TO  281
0471                  IF(((M.EQ.1).AND.(DEAVG.GT.0.0)).OR.((M.EQ.JE).AND.(DEAVG.LT.0.0))
                     X) DNAVG=-DEAVG*FNE(M)*0.5/EDE(M)
0472                   IF ((DEAVG.LT.0.0).AND.((M+1).LE.JE)) DNAVG=-DEAVG*(FNE(M+1)-FNE(M
                     X))/(EG(M+1)-EG(M))
0473                   IF ((DEAVG.GT.0.).AND.(M.GT.1)) DNAVG=DEAVG*(FNE(M)-FNE(M-1))/(EG(
                     XM)-EG(M-1))
0474               281 WRITE(6,182) M,FNE(M),FLX1,EG(M),CNE(M),EDE(M),FLX2 , DNAVG
0475               182 FORMAT(' ',I3,E12.5,5X,E12.4, 5X, F12.6,8X, E12.5,6X, F12.6,4X,E12
                     X.5,4X,E12.4)
0476                  DET=DDEG/ETV
0477                  WRITE(6,183) NTPP, N5TPN,NTPW ,DET, DAVGD, NCOL
0478               183 FORMAT(' ',//,3X,'TOTAL # OF PARTICLES PROCESSED =',I5,5X,'CUMULAT
                     1ED # OF PARTICLES =',I10,3X,'WGTED TOTL # OF PARTICLES=',F12.3,//,
                     X' NEW DT=',E12.5,4X,'OLD DAVG=',F12.5,4X,'# OF COLLISIONS=',I5,//)
0479                  WRITE(6,187)
0480               187 FORMAT(' '   ,1X, 'ZONE NUMBER', 5X, 'AVERAGE ENERGY',5X,'NUMBER O
                     1F ELECTRONS',3X,'CUMULATIVE # DEN(Z)',3X,'CUMU. AVG ENERGY',3X,
                     1'ZONE # DENSITY',/)
0481                  DO 282  M=1, JZ
0482                  ANZ=CNREZ(M)*AN5TP*DI5G
0483                  PCZ=CEZ(M)/CNREZ(M)
0484               282 WRITE(6,184) M, EZ(M), NREZ(M), ANZ, PCZ,FNREZ(M)
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0485          184 FORMAT(' ', 5X, I5, 5X, F14.6,8X,F14.6,  5X, F14.5, 7X,F14.6,7X,
                 1F12.5)
0486              WRITE(6,185)  NION,WNIZN,NIZN, ANIZVG,WNES, NES,ANES, WNAS,NAS,
                 XANAS, NTP, K1, K2, WF,BF
0487          185 FORMAT('0', 'NUMBER OF POSITIVE ION=',E14.6,//,' NUMBER OF IONIZAT
                 1IONS OCCURED=',F9.3,5X,'ACTUAL #=',I5,3X,'CUMULATIVE AVG=' ,F10.3,
                 X//,' # OF ESCAPED PARTICLES=',F9.3,5X,'ACTUAL#=',I5,3X,'CUMULATIVE
                 X AVG=',F9.2,//,' # OF ABSORPED PARTIC=',E12.4,3X,'ACTUAL #=',I5,3X
                 X,'CUMULATIVE AVG=',F9.2,//, ' TOTAL # OF PARTICLES IN THE NEW CYCL
                 XE =',I5,//,' K1=',I2, 3X,'K2=',I2,     4X,' BALANCE   FACTOR WF=',
                 XF10.5,3X,'BF2=', F10.5,/)
0488              WRITE(6,188) ED1, NPM, ND, KELC
0489          188 FORMAT(' ENERGY DIVIDING LINE FOR  RR PLAY E=',F10.4,4X,'EVERY',I2
                 X,'TH CYCLE CHANGE N+',//,' TIME INTERVAL MULTIPLY FACTOR=',F9.4,
                 X3X, 'ELASTIC XSEC / BY',I2,/)
0490              NDR=NDN-NDN/K3
0491              WRITE(6,186) NSO, NSW, ANSVG,NDR,WNSE,WNMET,ANMET,WNEXC,ANEXC,NUP,
                 XWGHT
0492          186 FORMAT(' ',   ' SOURCE PARTICLES GENERATED OLD =',I10,//,
                 1' SOURCE PARTICLES (WEIGHTED) IN THE NEW CYCLE =',I10,3X, 'CUMULAT
                 XIVE AVG=',F10.3,//
                 1,' # OF PARTICLES KILLED OFF IN RR PROC=',I10,//,
                 1' # OF SUPER ELASTIC COLLISION=',F10.4,//,
                 1                 ' # OF EXCITATIONS TO META STABLE LEVEL='
                 X,F10.4, 3X, 'CUMULATIVE AVG=', F9.3,
                 1                 //,' # OF EXCITATIONS TO OTHER LEVELS=',F10.4,
                 X4X, 'CUMULATIVE AVG=',F9.2,//,' # OF PARTICLES CROSS OVER TO HIGH
                 XENERGY REGION NUP=',I5,4X,'OVERALL WT=',E12.4,/)
0493              WRITE(6,195)  EF, EDP, PDPO ,SF1, SF2, SF3
0494          195 FORMAT (' E-FIELD=', F9.2,'V/CM', 4X,'E/P=',F9.2,4X,'P/PO =',F7.1,
                 X3X, 'SF1=', E12.4,3X, 'SF2=',E12.4,3X, 'SF3=', E12.4,/)
0495              WRITE(6,170) SO,WVC,SWFO,WVALUE,WVLE1, WVLE2,ESAVG, AESAVG,EASAVG,
                 XAEASG
0496          170 FORMAT(' SOURCE RATE =',E11.3,' PER SEC',4X,'W-VALUE(LOCAL  )=',
                 XF10.3, 3X,'SOURCE RED.FACT=',E13.4,//,' W-VALUE=',
                 XF10.3,4X,'CUM AVG WV1=',F9.3,3X,'CUM AVG WV2=',F9.3,
                 1       //,' AVERAGE ENERGY OF ESCAPED PARTICLES=',F12.5,3X,'CUMULAT
                 XIVE AVG=',F11.4,//,' AVERAGE ENERGY OF ABSORPED PARTICLES=',F12.5,
                 X3X, 'CUMULATIVE AVG=',F11.4,/ )
0497              CKFNE=SUMNE*ANTPO
0498              WRITE(6,189)CKFNE, CESUM, TNION, TNIO2
0499          189 FORMAT(' ','THE SN # CHECK =',F12.4,3X,'THE CN # CHECK=',F12.4,//,
                 1' CALCULATED N+ USE F=',E14.6,3X,'CALC. N+ USE CN =',E14.6,3X, 'AR
                 XTIF CN+=',E14.6,//)
0500              IF  ((MOD(NT,5).NE.0).OR.(MOD(NT,10).EQ.0))  GO  TO  3
0501              WRITE(9) EAVG, DAVG, TME, NTW, NT, NTP, NION,DDEG, NSW,SWF, E, U
0502              WRITE(9) Z, WT ,ANIOS, SF3
0503              ENDFILE 9
0504              REWIND 9
0505            3 CONTINUE
0506              IF  (MOD(NT,10).NE.0)  GO  TO  4
0507              WRITE(10) EAVG, DAVG, TME, NTW, NT, NTP, NION, DDEG, NSW,SWF, E, U
0508              WRITE(10) Z, WT  ,ANIOS, SF3
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0509                ENDFILE 10
0510                REWIND 10
0511              4 CONTINUE
0512                IF (MOD(NT,NCUM).NE.0)  GO  TO  6666
0513                N5TP=0
0514                NIP5=0
0515                D5AVS=0.0
0516                NAST=0
0517                NIZNT=0
0518                W5VLE=0.0
0519                CN5IZ=0.0
0520                CN5S=0.0
0521                CNMET=0.0
0522                CNEXC=0.0
0523                CESAVG=0.0
0524                CEASG=0.0
0525                CSF2=0.0
0526                CLOSS=0.0
0527                CNIO2=0.0
0528                CSF1=0.0
0529                DO  54  M=1,JZ
0530                CNREZ(M)=0.0
0531             54 CEZ(M)=0.0
0532                DO  55  M=1,JE
0533                TNE(M)=0.
0534             55 CNE(M)=0.0
0535                CNES=0.0
0536                CNAS=0.0
0537                DTAVS=0.0
0538                CETEP=0.0
0539                CETAS=0.0
0540                IF (MOD(NT,10).NE.0)  GO  TO  6666
0541           6666 CONTINUE
0542                NT= NT + 1
0543                DO  56  M=1,500
0544                DIZN(M)=0.0
0545                IES(M)=0
0546                IRR(M)=0
0547             56 IAS(M)=0
0548                DO  51  N=1,50
0549                WSE(N)=0.0
0550             51 ESE(N)=0.0
0551                I=1
                 C  REINITIALIZE THE OUTPUT QUANTITIES
0552                DO  52  M=1, JE
0553                EE(M)=0.
0554             52 NE(M)= 0.0
0555                DO  53  M=1,JZ
0556                NREZ(M)= 0.0
0557                EZ(M)=0.0
0558                DO  53  N=1,JE
0559                EKZ(N,M)=0.0
0560             53 NEZ(N,M)=0.0
```

```
FORTRAN IV G LEVEL  18                  MAIN                    DATE = 72126          05/31/02

0561                NIZN=0
0562                NOZN=0
0563                NIN=0
0564                NES=0
0565                NSE=0
0566                NCOL=0
0567                NAS=0
0568                NASW1=0
0569                DTOT=0.0
0570                NMET=0
0571                NEXC=0
0572                WNES=0.0
0573                WNAS=0.0
0574                WNEXC=0.0
0575                WNIZN=0.0
0576                WNMET=0.0
0577                WNSE=0.0
0578                ETAS=0.0
0579                ETEP=0.0
0580                ETOT=0.0
0581                NW=0
0582                NUP=0
0583                NDN=0
0584                NDNR=0
0585                INIV=INIV+ 1100
0586                CALL    RN3INZ(INIV)
0587                WRITE(6,72)
0588                IF (NT.LE.NTC)  GO  TO  7777
0589           9999 STOP
0590                DEBUG  SUBCHK
0591                END
```

```
FORTRAN IV G LEVEL  18                  INDEXE                  DATE = 72126          05/31/02

0001                  FUNCTION  INDEXE(E)
0002                  COMMON /AREA4/  CONST,DEL2, ELT,IE, DI1, DI2, DI3 ,DELI
0003                  IF (E.LT.0.08)  GO  TO  11
0004                  IF (E.GT.158.1335 ) GO  TO  13
0005               12 INDEXE= 5+(ALOG(E)*CONST +4.01*DI2
0006                  RETURN
0007               11 INDEXE=1 + E*DI1
0008                  RETURN
0009               13 INDEXE=36 + (ALOG(E)*CONST-7.005)*DI3
0010                  RETURN
0011                  END
```

```
FORTRAN IV G LEVEL  18                  SORCE2            DATE = 72126          09/31/12

0001                  SUBROUTINE  SORCE2(NSO, EAVG, NTW,PM, FID)
0002                  REAL  NI(55),FID(50) ,WI(55)
0003                  COMMON D, E(5100),Z(5100), U(5100) ,IAS(500),IRR(850),NRR,IFS(600)
                     X,WT(5100),SWF
0004                  COMMON /AREA2/ C1,MUO,EI,EIS,SF,ANEAM,PDPO,PI,EC,NION,JF,JZ,NASW1,
                     1NSEW ,AKT, AIKT ,AM1 ,AMC1,EDI,PDMUO, PD26,K1, K2, K3, WN2,EDP,EDN
0005                  COMMON /A5/ EG(55), EDE(55), EBD(55)
0006                  EM1(E)= EXP(-E*AIKT)*SQRT(E)*AM1
0007                  EM2(E)=AA/E
0008                  EM3(E)=EXP(-E*AIKT)*SQRT(E) *AMC1
0009                  REAL  MUO, NION
0010              604 FORMAT(' ',F12.6,3X, I3, 3X, E12.4, 2X, F12.6,2X,F12.5,3X,E12.4)
0011              605 FORMAT(' ','J1=',I3,3X,'EDI=',F9.3,      3X,'NSO=',I8,3X,'K1=',
                     1I8,3X,'K2=',I8,//,' INITIAL DISTRIBUTION',//,' # OF PTS',7X,'INDEX
                     1',5X, '# DENSITY',4X,'AVG ENERGY',6X,'DEL-E',6X,'WEIGHT',/)
0012              606 FORMAT(' ','NS1=',I5,3X,'NS2=',I5,3X,'NSO=',I5,3X,'NTW=',I5,3X,
                     X'NTW(CALC)=',I5,//)
0013              607 FORMAT(' EAVG=', F12.5,3X,'WGHTED EAVG=',F12.5,//)
0014                  AA=2.0*PM*SQRT(PM/PI)*EXP(-PM)
0015                  J1=INDEXE(EDI-0.5)
0016                  J2=J1+1
0017                  ISUM=0
0018                  WRITE(6,605)   J1, EDI,NSO, K1, K2
0019                  DO  100  I=1,J1
0020                  ONI  =FIO(I)*EDE(I)*NTW/K1
0021                  NI(I)=ONI
0022                  WI(I)=1.0
0023                  IF (FID(I).LE.0.0)  GO  TO  112
0024                  IF (ONI.GT.200.)  NI(I)=200
0025                  IF (ONI.GT.200.)  WI(I)=ONI/200.
0026                  IF (ONI.LT.12)  NI(I)=12
0027                  IF (ONI.LT.12)  WI(I)=ONI/12.0
0028              112 WRITE(6,604) NI(I), I, FID(I),EG(I), EDE(I),WI(I)
0029              100 ISUM=ISUM+ NI(I)
0030                  JSUM=0
0031                  DO  200  I=J2, JE
0032                  ONI  =FIO(I)*EDE(I)*NTW*K2
0033                  NI(I)=ONI
0034                  WI(I)=1.0
0035                  IF (FID(I).LE.0.0)  GO  TO  202
0036                  IF (ONI.GT.200.)  NI(I)=200
0037                  IF (ONI.GT.200.)  WI(I)=ONI/200.
0038                  IF (ONI.LT.12)  NI(I)=12
0039                  IF (ONI.LT.12)  WI(I)=ONI/12.0
0040              202 WRITE(6,604) NI(I), I, FID(I),EG(I), EDE(I), WI(I)
0041              200 JSUM= JSUM + NI(I)
0042                  NSUM=ISUM+JSUM
0043                  NTW2=ISUM*K1 +JSUM*WN2 +0.5
0044                  WRITE(6,606) ISUM, JSUM, NSUM, NTW, NTW2
0045                  NTW=NTW2
0046                  IE=1
0047                  EAG=0.0
0048                  DO  300  I=1, JE
```

```
FORTRAN IV G LEVEL  18                  SORCE2          DATE = 72126          05/31/02

0049              IF  (NI(I).LT.1)  GO  TO  300
0050               JI=NI(I) +IE -1
0051               DO  301  J=IE, JI, 2
0052              RI=RAN3Z(0)
0053              R2=1.0-RI
0054              E(J)= EBD(I) + EDE(I)*RI
0055              E(J+1)= EBD(I) + EDE(I)*R2
0056              WT(J)=WI(I)
0057              WT(J+1)=WI(I)
0058              EAG =EAG + E(J) +E(J+1)
0059              IF((MOD((JI-IE),2).EQ.0).AND.(J.GE.JI)) EAG=EAG-E(J+1)
0060          301 CONTINUE
0061              IE=IE+NI(I)
0062          300 CONTINUE
0063              NSO=NSUM
0064              EAVG=EAG/NSO
0065              I2=NSO
0066              ETW=0.0
0067              DO  400  I=1,NSO
0068              IF  (E(I).LE.ED1) WT(I)=K1 *WT(I)
0069              IF  (E(I).GT.ED1) WT(I)=WN2*WT(I)
0070              IF (E(I).LE.0.0)  E(I)=E(I-1)
0071              ETW=ETW + E(I)*WT(I)
0072          400 CONTINUE
0073              EWAVG=ETW/NTW2
0074              WRITE(6,607) EAVG, EWAVG
0075              QDZ=D*0.25
0076              I=1
0077          101 RZ=RAN3Z(0)
0078              RU=RAN3Z(0)
0079              Z(I)=D*RZ
0080              U(I)=2.0*RU -1.0
0081              I= I+ 1
0082          102 Z(I)=D*RZ
0083              U(I)=1.0- 2.0*RU
0084              I= I +1
0085          103 Z(I)=D*(1.0-RZ)
0086              U(I)= 2.0*RZ-1.0
0087              I= I +1
0088          104 Z(I)=D*(1.0-RZ)
0089              U(I)= 1.-2.*RZ
0090              I= I+ 1
0091              IF((I2 -I-3).GE.0)  GO  TO  101
0092              IF (I2.LT.I)  GO  TO  105
0093              RZ=RAN3Z(0)
0094              RU=RAN3Z(0)
0095              IF((I2 -I).EQ.2)  GO  TO   102
0096              IF((I2 -I).EQ.1)  GO  TO  103
0097              IF((I2 -I).EQ.0)  GO  TO  104
0098          105 RETURN
0099              END
```

```
FORTRAN IV G LEVEL  18                  SOURCE              DATE = 72126          05/31/02

0001                  SUBROUTINE  SOURCE(NS,NTP)
0002                  COMMON D, E(5100),Z(5100), U(5100) ,IAS(500),IRR(850),NRR,IES(600)
                     X,WT(5100),SWF
0003                  COMMON /AREA2/ C1,MUO,EI,EIS,SF,ANEAM,PDPO,PI,EO,NION,JE,JZ,NASW1,
                     1NSEW ,AKT, AIKT ,AM1 ,AMC1,ED1,PDMUO, PD26,K1, K2, K3, WN2,ED2,ED3
0004                  REAL  MUO, NION
                C SOURCE PARTICLE PARAMETERS GENERATING PROCEDURE
                C I1: THE INITIAL INDEX VALUE FOR THE SOURCE PARTICLE
0005                  I=NTP+1
0006                  DO  100  K=1, NS, 2
0007                  E(I)=EO
0008                  RZ=RAN3Z(0)
0009                  RU=RAN3Z(0)
0010                  Z(I)=D*RZ
0011                  U(I)=RU+RU-1.0
0012                  WT(I)=WN2/SWF
0013                  IF  ((NS-K).LE.0)  GO  TO  100
0014                  E(I+1)=EO
0015                  Z(I+1)= RZ*D
0016                  U(I+1)=-U(I)
0017                  WT(I+1)=WN2/SWF
0018                   I=I+2
0019                100 CONTINUE
0020                  NTP=NTP+NS
0021                105 RETURN
0022                  END
```

```
FORTRAN IV G LEVEL  18                  MAIN                DATE = 72126        05/31/02

      C WHENEVER THERE ARE MORE HOLES THAN SOURCE PARTICLES, FILL IN THE EXTRA HOLES W
      C WITH PARTICLES AT THE END
0001        SUBROUTINE   FILHOL(NTP, NES, NAS)
0002        COMMON D, E(5100),Z(5100), U(5100) ,IAS(500),IRR(850),NRR,IES(600)
           X,WT(5100),SWF
0003        K=NTP
0004        IF (NES.LE.0)  GO  TO  105
0005        DO  100  I=1, NES
0006        J=IES(I)
0007        E(J)= E(K)
0008        Z(J)= Z(K)
0009        U(J)= U(K)
0010        WT(J)=WT(K)
0011      100 K=K-1
0012        NTP=NTP-NES
0013      105 IF (NAS.LE.0)  RETURN
0014        K=NTP
0015        DO  300  I=1,NAS
0016        J=IAS(I)
0017        E(J)=E(K)
0018        Z(J)=Z(K)
0019        U(J)=U(K)
0020        WT(J)=WT(K)
0021      300 K=K-1
0022        NTP=NTP-NAS
0023      200 RETURN
0024        END
```

```
FORTRAN IV G LEVEL  18                  RRPROC              DATE = 72126          05/31/02

0001              SUBROUTINE  RRPROC(NTP,K3)
0002              COMMON D, E(5100),Z(5100), U(5100) ,IAS(500),IRR(850),NRR,IES(600)
                 X,WT(5100),SWF
0003              COMMON /A6/ ESE(50) , NUP ,NDNR,NDN, WSE(50)
0004              NR=NDNR
0005              K=NTP
0006              IF (K3.LE.1)   RETURN
0007           100 CONTINUE
0008              I=IRR(NR)
0009              E(I)=E(K)
0010              U(I)=U(K)
0011              Z(I)=Z(K)
0012              WT(I)=WT(K)
0013              K=K-1
0014           200 NR=NR-1
0015              IF  (NR.GT.0)  GO  TO  100
0016              NTP=K+1
0017           300 RETURN
0018              END
```

```
FORTRAN IV G LEVEL  18                ALDA                DATE = 72126          05/31/02

0001                FUNCTION  ALDA(E)
0002                COMMON /AREA2/ C1,MUO,EI,EIS,SF,ANEAM,PDPO,PI,EO,NION,JE,JZ,NASW1,
                   1NSEW ,AKT, AIKT ,AM1 ,AMC1,ED1,PDMUO, PD26,K1, K2, K3, WN2,ED2,ED3
0003                COMMON /AREA3/ XSEL,XELC,XRCB,XMET,XEXC,XION,XTOL,KELC
0004                REAL  MUO, NION
0005                WELC=1.0/KELC
0006                IF (E.LE.5.)  XELC=23.0*PDPO
0007                IF((E.GT.5.).AND.(E.LE.19.8))  XELC=23.0*PDPO*SQRT(5./E)
0008                IF (E.GT.19.8)  XELC=EXP(-0.02*E)*16.76*PDPO
0009                XELC=XELC*WELC
0010                IF (E.LE.ED3 )  GO  TO  5001
0011           4001 AE1= 0.25 +(E    - 19.80)**2
0012                XMET= 0.109*(E    -19.80)/AE1 + 0.0311
0013                XMET=XMET*PDPO
0014                E19= E - 21.4
0015                AE2= 1850. + E19**2
0016                XEXC= 68.80*E19*PDPO/AE2
0017                IF (E.LT.21.4)  XEXC=0.0
0018                E24= E - EI
0019                AE3= 4900. + E24**2
0020                XION= 172.*E24/AE3
0021                XION=XION*PDPO
0022                IF  (E.LT.24.46)  XION=0.0
0023                XTOL= XMET +XEXC +XION +XELC
0024                XRCB=0.0
0025                XSEL=0.0
0026                GO  TO  6001
0027           5001 BE1=0.250+ (E-19.8)**2
0028                XSEL=0.109*(19.8 -E    )/BE1
0029                XSEL=XSEL*PDPO*ANEAM
0030                XRCB=PDMUO*NION/SQRT(E)
0031                XION=0.0
0032                XEXC=0.0
0033                XMET=0.0
0034                XTOL= XSEL +XELC +XRCB
0035           6001 ALDA=1.0/XTOL
0036                RETURN
0037                END
```

```
FORTRAN IV G LEVEL  18                  COLPRO              DATE = 72126          05/31/02

0001                  SUBROUTINE   COLPRO(I, DCEN, NTP, RIP, NUST, *, *)
0002                  COMMON D, E(5100),Z(5100), U(5100) ,IAS(500),IRR(850),NRR,IES(600)
                     X,WT(5100),SWF
0003                  COMMON /AREA1/ NIZN, NOZN, NAS, DIZN(500),NSE, NMET, NEXC, ETAS  ,
                     XWNMET, WNEXC, WNIZN, ELS,WNAS ,WNSE
0004                  COMMON /AREA2/ C1,MUO,EI,EIS,SF,ANEAM,PDPO,PI,EO,NION,JE,JZ,NASW1,
                     1NSEW ,AKT, AIKT ,AM1 ,AMC1,ED1,PDMUO, PD26,K1, K2, K3, WN2,ED2,ED3
0005                  COMMON /AREA3/ XSEL,XELC,XRCB,XMET,XEXC,XION,XTOL,KELC
0006                  COMMON /A6/ ESE(50) , NUP ,NONR,NON, WSE(50)
0007                  DIMENSION  PX(4)
0008                  FM3(E)=EXP(-E*AIKT)*SQRT(E)*AMC1
0009                  REAL  MUO, NION
                    C DECIDE WHICH KIND OF COLLISION
0010                  XTI =ALDA(E(I))
0011                  IF (E(I).LE.ED3 )  GO  TO  5000
                    C  ENERGY REGION 1  19.0EV  TO  1 KEV
0012                4000 PMET= XMET*XTI
0013                  PEXC= XEXC*XTI
0014                  PION= XION*XTI
0015                  PELC=XELC*XTI
0016                  PX(1)= PEXC
0017                  PX(2)= PEXC +PMET
0018                  PX(3)= PX(2) +PION
0019                  IP=1
0020                  DO  45  IX=1,3
0021                 45 IF(RIP.GT.PX(IX))  IP=IX+1
0022                  GO  TO  (4015,4013,4017,4011), IP
0023                4011 R1=RAN3Z(0)
0024                  U(I)= 2.0*R1 -1.0
0025                  RETURN
                    C INELASTIC COLLISION PROCESS EXCITE TO META STABLE STATE
                    C EXCITATION TO METASTABLE LEVEL
0026                4013 WNMET= WNMET +WT(I)
0027                  E(I)= E(I) - 19.80
0028                  IF (E(I).LE.0.0)  RETURN1
0029                  NMET=NMET+1
0030                  RI1= RAN3Z(0)
0031                  U(I) = RI1 +RI1 - 1.0
0032                  RETURN
                    C EXCITION TO OTHER LEVELS
0033                4015 WNEXC =WNEXC +WT(I)
0034                  E(I)= E(I) -21.40
0035                  IF (E(I).LE.0.0)  RETURN1
0036                  NEXC=NEXC+1
0037                  RI1= RAN3Z(0)
0038                  U(I) = RI1 +RI1 - 1.0
0039                  RETURN
                    C IONIZITION PROCESS  PRODUCE SECONDRY ELECTIONS
0040                4017  WNIZN= WNIZN+ WT(I)
0041                  E(I)= E(I) - EI
0042                  IF (E(I).LE.0.0)  RETURN1
0043                  NIZN=NIZN+1
0044                  NOZN=NOZN   +1
```

```
FORTRAN IV G LEVEL  18                  COLPRO              DATE = 72126          05/31/02
C IONIZATION PRODUCED PARTICLES ALWAYS PUT TO THE END OF RESIDUES
0045            DIZN(NOZN)= OCEN
0046            RI=RAN3Z(0)
0047            U(I)=RI+RI-1.0
0048            NNTP =NTP +NIZN
0049            E(NNTP)= E(I)*0.1
0050            Z(NNTP)=Z(I)
0051            U(NNTP)=-U(I)
0052            E(I)= E(I)*0.9
0053            WT(NNTP)= WT(I)
0054            IF ((E(NNTP)    .GT.ED1).OR.((E(I)*1.111+EI).LT.FD1))  GO  TO 4018
0055            NDN=NDN+1
0056            NDNR=NDNR+1
0057            WT(NNTP)=WT(I)*K3
0058            IRR(NDNR)=NTP+NIZN
0059         4018 CONTINUE
0060            RETURN
C ENERGY REGION 2 LOW ENERGY RANGE DOWN TO THERMAL REGION
0061         5000 PELC= XELC*XTI
0062            PSEL= XSEL*XTI
0063            PRCB= XRCB*XTI
0064            PX(1)= PRCB
0065            PX(2)= PSEL +PRCB
0066            IP=1
0067            DO  55  IX=1,2
0068              55 IF(RIP.GT.PX(IX))  IP=IX+1
0069            GO  TO  (5013,5015,5011),IP
C ELASTIC COLLISION PROCESS
0070         5011 IF (ELS.LE.0.0)  GO  TO  50125
0071            IF ((NUST.EQ.0).OR.(E(I).GT.2.5))  GO  TO  50124
0072         50115 RE=RAN3Z(0)
0073            R2=RAN3Z(0)
0074            E1=ED2*RE
0075            E2=ED2*R2
0076            FR1=FM3(E1)
0077            FR2=FM3(E2)
0078            IF  (RE.LE.FR2)  RS=RE
0079            IF  (R2.LE.FR1)  RS=R2
0080            IF  ((RE.LE.FR2).OR.(R2.LE.FR1))  GO  TO  5012
0081            GO  TO  50115
0082         5012 ENN=RS*ED2
0083         50124 IF((NUST.EQ.0).OR.(E(I).GT.2.5))  ENN=0.0
0084            R1=RAN3Z(0)
0085            U1=2.0*R1 -1.0
0086            UM=SQRT((1.-U1**2)*(1.-U(I)**2))
0087            US=2.0*RIP-1.0
0088            COSST=U1*U(I) +SIGN(UM,US)
0089            DELE=C1*(E(I)-ENN)*(1.0-COSST)*ELS*KELC
0090            E(I)= E(I) -DELE
0091            U(I)=U1
0092         50125 IF( ELS.LE.0.0)  U(I)= 2.0*RAN3Z(0) -1.0
0093            RETURN
C RECOMBINATION PROCESS
```

```
FORTRAN IV G LEVEL  18                  COLPRO              DATE = 72126          05/31/02

0094          5013 NAS=NAS+1
0095               IAS(NAS)=I
0096               WNAS= WNAS+WT(I)
0097               IF  (E(I).GT.0.0)  ETAS=ETAS+E(I)*WT(I)
0098               RETURN2
                 C SUPERELASTIC COLLISION PROCESS
0099          5015 E(I)= E(I) + EIS
0100               WNSE=WNSE +WT(I)
0101               NSE=NSE+1
0102               RP= RAN3Z(0)
0103               U(I)= RP +RP -1.0
0104               RETURN
0105               END
```

```
FORTRAN IV G LEVEL 18                MAIN                DATE = 72125          01/28/29

      C MASTER PROGRAM OF MONTE CARLO SIMULATION OF NONLINEAR ALPHA PLASMAS (ALPHA PAR
      C TICLES INDUCED PLASMA ELECTRON ENERGY DISTRIBUTION STUDY
      C DEFINITIONS AND TERMINOLOGY
      C D: DIAMETER OF THE CYLINDER THE LENGTH OF THE FINITE REGION
      C EO:INITIAL ENERGY OF THE SOURCE PARTICLES SO(NS): SOURCE RATE
      C JZ:TOTAL NUMBER OF ZONES   JE: TOTAL NUMBER OF ENERGY RANGES
      C IAS: ARRAY FOR STORING THE INDEX OF ABSORPED PARTICLES NAS: THE NO. OF THEM
      C DB: DISTANCE TO BOUNDRY  DCOL: DISTANCE TO COLLISION  DCEN: DISTANCE TO CENSUS
      C DZ: ZONE INTERVAL
      C ARRAYS E. Z. U  STORING ENERGY. DISTANCE. AND DIRECTION OF PARTICLES
      C NTP: TOTAL NUMBER OF PARTICLES TO BE PROCESSED  EACH CYCLE
      C NT: TOTAL NUMBER OF TIME CYCLES
      C NS: NUMBER OF SOURCE PARTICLES PER UNIT TIME*DISTANCE  OR SOURCE RATE
      C NIZN: NUMBER OF IONIZATION PROCESS OCCURRED EACH TIME CYCLE
0001            REAL    NE(55), NEZ( 55,10),EZ(11),DX(3),EE(55),  CEZ(11),EKZ(55
     1,10) ,FID(60),NREZ(11),EZI(11),NTPW
0002            DIMENSION  FNE(55), FNREZ(11), NRZI(11),CNE(55), CNREZ(11),TNE(55)
0003            COMMON D, E(5100),Z(5100), U(5100) ,IAS(500),IRR(850),NRP,IFS(600)
     X,WT(5100),SWF
0004            COMMON /AREA1/ NIZN, NOZN, NAS, DIZN(500),NSE, NMET, NEXC, ETAS  ,
     XWNMET, WNEXC, WNIZN, ELS,WNAS ,WNSE
0005            COMMON /AREA2/ C1,MUO,EI,EIS,SF,ANEAM,PDPO,PI,EO,NION,JE,JZ,NASW1,
     1NSEW ,AKT, AIKT ,AM1 ,AMC1,ED1,PDMUO, PD26,K1, K2, K3, WN2,ED2,ED3
0006            COMMON /AREA3/ XSEL,XELC,XRCB,XMET,XEXC,XION,XTOL,KELC
0007            COMMON /AREA4/  CONST,DEL2, ELT,IE, DI1, DI2, DI3 ,DELI
0008            COMMON /A5/ EG(55), EDE(55), EBD(55)
0009            COMMON /A6/ ESE(50) , NUP ,NONR,NDN, WSE(50)
0010            REAL  MUO, NION,ND
      C STATEMENT FUNCTION FOR EVALUATING  MAXWELLIAN AND RELATED FCNS
0011            FM1(E,FNEM)=EXP(-E*AIKT)*SQRT(E)*FNEM
0012            DATA  TMS,NT,DTOT,ETOT,NIN,NIZNT,NAST/0.0,1,0.0,0.0,0.0,0.0,0/
0013            DATA W5VLE,CN5IZ,CN5S,CNES,CNAS,CNMET,CNEXC,CESAVG,CEASG/9*0.0/
0014            DATA CNE/ 55*0.0/, CEZ/11*0.0/, CNREZ/11*0.0/,TNE/55*0./,EKZ/550*0
     1.0/,D5AVS/0.0/
0015            DATA NEZ/ 550*0./,NE/55*0./,EZ/11*0./,NREZ/11*0./,EE/55*0.0/
0016            READ(5,1) NTAPE
0017            READ(5,151) K1, K2, NTC, NTP,NTW,NPM, KELC ,JZ, IM,NCUM, NDPN,NTMP
     X, MC ,IUSN, NUST, NBF
0018            READ(5,152) ED1 ,ND , EO, ELS, D,ANSW, PDPO, SR
0019            READ(5,153) FID
0020          1 FORMAT ( I10)
0021        151 FORMAT( 16I5)
0022        152 FORMAT( 8F10.4)
0023        153 FORMAT( 8E10.3)
0024            AKT=0.05
0025            AIKT= 1.0/AKT
0026            PI=3.141593
0027            EMASSI=1.60203E+16/9.108
0028            K3=K1*K2
0029            WN2=1.0/K2
0030            CJD=0.0
0031            EI=24.46
0032            EIS=21.4
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0033                C1=2.*0.000549/4.003873
0034                ETV= SQRT(2.0*1.60203/9.1081*1.0E+08
0035                VTE= 1.0/(ETV*ETV)
0036                CALL  UNDERZ('OFF')
0037                PD26=PDP0*26.0
0038                MU0=(1.0E+09)/ETV
0039                CMU0=1.0E-09
0040                CMUPDP=CMU0*PDP0
0041                IF (PDP0.GT.10.0)  CMUPDP=CMU0*10.0
0042                PDMU0=CMUPDP/ETV
0043                CLOSS=0.0
0044                NUP=0
0045                NDN=0
0046                NDNP=0
0047                IN0=0
0048                NRR=0
0049                NAS=0
0050                NES=0
0051                NSE=0
0052                NOZN=0
0053                NIZN=0
0054                NIN=0
0055                LK=0
0056                INIV=999999
0057                NMET=0
0058                NEXC=0
0059                ETAS=0.0
0060                ETEP=0.0
0061                NTP5=0
0062                NW=0
0063                N5TP=0
0064                DTAVS=0.0
0065                CSF2=0.0
0066                CNIO2=0.0
0067                CSF1=0.0
0068                CETAS=0.0
0069                CETEP=0.0
0070                NCOL=0
0071                WNMET=0.0
0072                WNSE=0.0
0073                WNEXC=0.0
0074                WNES=0.0
0075                WNAS=0.0
0076                WNIZN=0.0
0077                JE=48
0078                IE=JE
0079                DEN=3.54E+16*PDP0
0080                DETZ=D/JZ
0081                DZIV= 1.0/DETZ
0082                CONST=1.0/ALOG(2.0)
0083                ED2=0.447513
0084                ED3=19.8
0085                PM=ED2*AIKT
```

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0086                AM1=2.0*AIKT/SQRT(PI*AKT)
0087                CALL   RN3INZ(994563211)
0088                SO=PUPO*SR*1.0E+16
0089                AITG=  CMUPOP /(AKT*PI)
0090                DE1=0.016
0091                DE2=0.355
0092                DE3=0.3
0093                DI1=1./0.016
0094                DI2=1./DE2
0095                DI3=1./DE3
0096                AMC1= SQRT(2.0*2.7183*AIKT)*ED2
0097                DO  11  I=6, 36
0098                EBL =(I-5)*DE2 -4.0
0099                EMV= EBL -0.1685
0100                EBD(I)= 2.0**EBL
0101                EG(I-1)= 2.0**EMV
0102             11 EDE(I)=EBD(I)*(2.0**DE2 -1.0)
0103                JE1=JE+1
0104                DO  12  I=37, JE1
0105                EBL= 7.005 +(I-36)*DE3
0106                EMV= EBL - 0.1405
0107                EBD(I)= 2.0**EBL
0108                EG(I-1)= 2.0**EMV
0109             12 EDE(I)= EBD(I)*(2.0**DE3 -1.0)
0110                DO  10  I=1, 5
0111                EDE(I)= 0.016
0112                EG(I)= EDE(I)*I -0.008
0113             10 EBD(I)= EDE(I)*(I-1)
0114                EDE(36)=29.69
0115                EG(48)= 1737.482
0116                IF  (NTAPE.NE.1)  GO  TO  2
0117                READ(10)  EAVG, DAVG, TME, NTW, NT, NTP, NION, DDEG, NSW,SWF, E,U
0118                READ(10) Z, WT, ANIOS,SF3
0119                NS=NSW*K2
0120                REWIND  10
0121                NT=NT+1
0122             2  CONTINUE
0123                IF (NTAPE.NE.2)  GO  TO  5
0124                READ(9 )  EAVG, DAVG, TME, NTW, NT, NTP, NION, DDEG, NSW,SWF, E, U
0125                READ(9 ) Z, WT, ANIOS,SF3
0126                NS=NSW*K2
0127                REWIND  9
0128                NT=NT+1
0129             5  CONTINUE
0130                IF  (NTAPE.NE.0)  GO  TO  122
0131                NION= SQRT(SO*10/AITG)
0132                 ANEAM=NION*0.33333/DEN
0133                CALL  SORCE2(NTP, EAVG, NTW, PM, FID)
0134                AL=ALDA(EAVG)
0135                DAVG=AL
0136                DDEG=DAVG*ND/SQRT(EAVG)
0137                 SF2=1.0
0138                IF  (NION.NE.0)  SF2=NTW/NION
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0139                SN=SO*AL*ND*SF2/(ETV*SQRT(EAVG))
0140                NSW=ANSW+0.5
0141                IF (SN.GT.ANSW) NSW=SN +0.5
0142                NS=NSW*K2
0143                SWF=NSW/SN
0144                SF=SWF
0145                ANIOS=NICN
0146                CALL  SOURCE(NS,NTP)
0147                SF1=SF2
0148                SF3=SF2
0149                TME=0.C
0150              122 CONTINUE
0151                SF=SWF
                C  GENERATE SOURCE PARTICLES TO INITIALIZE THE PROGRAM
0152                ANEAM=NION*0.33333/DEN
0153                WRITE(6,70)
0154               70 FORMAT('1','PROGRAM INITIALIZATION AND THE INITIAL PARAMETERS',//)
0155                WRITE(6,71) AITG, NION, NTP, AL,EAVG
0156               71 FORMAT(' ', 'AITG =',E14.6, 3X,'NION =',E14.6,3X,'NTP =',I12,3X,
                   1'DCEN(EO) =', F14.6,3X, 'EAVG= ',F14.4,/)
0157               72 FORMAT(' ',8X,'DCOL',13X,'DCEN',13X,'ENERGY',11X,'Z',14X,'U', 10X,
                   X'WEIGHT',/)
0158               75 FORMAT(' ',F14.6,3X, F14.6, 3X, F14.5,3X, F12.4,3X,F12.4,3X,F13.4)
0159                WRITE(6,72)
0160                RIP=RAN3Z(0)
0161                I=1
                C WITHIN THE OUTER I LOOP THE I TH PARTICLE HISTORY
                C  GEOMETRIC ROUTINE ENTERING HERE
0162             7777 IF ((E(I).LE.0.0).OR.(E(I).GT.EO)) GO TO 9008
0163                DCEN=DDEG*SQRT(E(I))
0164             7778 IF ((NIZN.GT.0).AND.(I.GT.NTP)) DCEN= DIZN(NOZN+1)
0165                NFLG=0
0166                U(I)=U(I)*IUSN
0167                LFG2=0
0168                ETAG1=1.0
0169                IF (E(I).GT.ED1) ETAG1=-1.0
0170             3000 IF ((Z(I).LE.0.0).OR.(Z(I).GT.D).OR.(E(I).LE.0.0)) GO TO 9008
0171                J=INT(Z(I)*DZIV) +1
0172                RI=RAN3Z(0)
0173                ALD=ALDA(E(I))
0174                DCOL=ALD*ABS(ALOG(RI))
0175                IF (NFLG.EQ.1) GO TO 809
0176                IF(MOD(I,IM).EQ.0) WRITE(6,75)  DCOL,DCEN,E(I),Z(I),U(I),WT(I)
0177                DCOL2=ABS(ALOG(1.-RI))*ALD
0178                DTOT=DTOT +DCOL+DCOL2
0179                ETOT=ETOT+E(I)
0180                IF (NDPN.LT.2) GO TO 809
0181                DCEN2=DCEN
0182                EIO=E(I)
0183                UIO= U(I)*IUSN
0184                ZIO=Z(I)
0185              809 NFLG=1
0186              900 IF (DCEN.LT.DCOL) GO TO 902
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0187          901 DCEN=DCEN- DCOL
0188              Z(I)=Z(I) +DCOL*U(I)
0189              NCOL=NCOL+1
0190              IF (MOD(NCOL,MC).EQ.0) RIP=RAN3Z(0)
0191              IF (MOD(NCOL,MC).NE.0) RIP=1.0-RIP
0192              CALL  COLPRO(I, DCEN, NTP, RIP, NUST, &9008, &9009)
0193              GO  TO  3000
0194          902 Z(I)= Z(I) +DCEN*U(I)
0195               IF ((Z(I).LE.0.0).OR.(Z(I).GT.D))  GO  TO  9008
0196              J=INT(Z(I)*DZIV)+1
0197              IF (J.GT.JZ)  J=JZ
0198              K= INDEXE(E(I))
0199              IF (K.GT.JE) K=JE
0200              IF (K3.EQ.1)  GO  TO  904
0201              ETAG2=1.0
0202              IF (E(I).GT.ED1)  ETAG2=-1.0
0203              IF ((ETAG1*ETAG2).GT.0.0)  GO  TO  904
0204              IF (ETAG2.GT.0.0)  GO  TO  903
0205              NUP=NUP+1
0206              ESE(NUP)=E(I)
0207              WT(I)=WT(I)/K3
0208              WSE(NUP)=WT(I)
0209              GO  TO  904
0210          903 IF((LFG2.EQ.1).OR.(NDPN.LT.2))  NDNR=NONR+1
0211              IF((LFG2.EQ.1).OR.(NDPN.LT.2))  IRR(NDNR)=I
0212              NON=NON+1
0213              IF (MOD(NON,K3).NE.0)  GO  TO  9045
0214              WT(I)=WT(I)*K3
0215          904 NEZ(K,J)= NEZ(K,J) + WT(I)
0216              EKZ(K,J)=EKZ(K,J)+E(I)*WT(I)
0217         9045 IF((LFG2.EQ.1).OR.(NDPN.LT.2))  GO  TO  9009
0218              LFG2=1
0219              E(I)=EIO
0220              U(I)=UIO
0221              Z(I)=ZIO
0222              DCEN=DCEN2
0223              DCOL=DCOL2
0224              GO  TO  900
0225         9008 NES=NES+1
0226              IF (E(I).LT.ED1) WT(I)=WT(I)/K3
0227              WNES=WNES +WT(I)
0228              IES(NES)=I
0229              IF  (E(I).GT.0.0)  ETEP=ETEP+E(I)*WT(I)
0230         9009 I= I+1
0231              LFG2=0
0232              IF (I.LE.NTP)  GO  TO  7777
0233              IF ((I.GT.NTP).AND.(NIZN.GT.0))  NOZN= NOZN-1
0234              IF (NOZN.LT.0)  NIN=1
0235              IF ((NIZN.GT.0) .AND.(NIN.EQ.0))  GO  TO  7778
0236              NIZW=WNIZN +0.5
0237              NWS=WNES +0.5
0238              NASW=WNAS  +0.5
0239              WNAS=WNAS/KELC
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0240                WNSE=WNSE/KELC
0241                NSEW=WNSE +0.5
0242                DO  191  M=1,JE
0243                DO  191  N=1,JZ
0244                EE(M)=EE(M) + EKZ(M,N)
0245              191 NE(M)= NE(M) + NEZ(M,N)
0246                IF ((K3.EQ.1).OR.(NUP.EQ.0))  GO  TO  24
0247                 N3=K3/JZ
0248                IF   (N3.LT.1)  M3=1
0249                NK3=K3-1
0250                IF (NK3.LT.JZ) IZ=NK3
0251                 IF (N3.GE.1)  M3=N3
0252                DO  23  N=1,NUP
0253                K=INDEXE(ESE(N))
0254                EE(K)=EE(K) + (K3-1)*ESE(N)*WSE(N)
0255                NE(K)=NE(K) +(K3-1)*WSE(N)
0256             22 IF (NK3.GE.JZ)  IZ=JZ
0257                DO  21  L=1,IZ
0258                NREZ(L)=NREZ(L) + M3*WSF(N)
0259             21 EZ(L)=EZ(L) + ESE(N)*M3*WSE(N)
0260                NK3=NK3 -JZ*M3
0261                IF (NK3.LT.JZ)  IZ=NK3
0262                M3=1
0263                IF (NK3.GT.0)  GO  TO  22
0264             23 CONTINUE
0265             24 CONTINUE
0266                DO  192  M=1, JZ
0267                DO  1915  N=1,JE
0268                NREZ(M)=NREZ(M) + NEZ(N,M)
0269           1915 EZ(M)=EZ(M) +EKZ(N,M)
0270            192 CONTINUE
0271                NTPN=NTP+NIZN-NES-NAS
0272                NTPW=0.0
0273                ETOL=0.0
0274                DO  14  M=1,JE
0275                ETOL= ETOL +EE(M)
0276             14 NTPW=NTPW +NE(M)
0277                EWTOL=ETOL
0278                NTPT=NTPN
0279                DAVGO= DAVG*ND
0280                DAVS=(DAVGO*1000.)**NTMP
0281                D5AVS=D5AVS+ DAVS
0282                D15G=1.2/D5AVS
0283                ANTPO = 1.0/NTPW
0284                N5TP= N5TP + NTPW +0.5
0285                DTAVS=DTAVS +DAVS
0286                NTP5=NTP5+ NTPN*DAVS
0287                NTPO=NTP
0288                EWAVG=EWTOL*ANTPO
0289                NSO=NS
0290                NSWO=NSO*WN2 +0.5
0291                NTP=NTP+NIZN
0292                NTPP=NTP
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0293                  DAVG=DTOT*0.5/NTP
0294                  EAVG= ETOT/NTP
0295                  DEG=DDEG/ETV
0296                  TMF=TME+DEG
0297                  TMS=TMS+DEG
                C IF SOURCE PARTICLES SO(NS)< NES THEN ELIMINATE AS MANY RESIDUE PARTICLES AT TH
0298                  NTPS=NTPW + NWS +NASW
0299                  DCEN1= ALOA( EAVG)
0300                  NTW=NTPW +.5
0301                  DDEG=DAVG*ND/SQRT( EAVG)
0302                  SF2=1.0
0303                  IF (ANIOS.NE.0)  SF2=NTPS/ANIOS
0304                  ESAVG=0.0
0305                  IF(WNES.NE.0.0)  ESAVG= ETEP/WNES
0306                  EASAVG=0.0
0307                  IF (WNAS.NE.0)  EASAVG=ETAS/WNAS
0308                  SWF0=SWF
0309                  BF=1.0
0310                  IF  ((WNES+WNAS).GT.0.0)  BF=(WNIZN+SN)/(WNES+WNAS)
0311                  CN5S=CN5S+ SN*DAVS
0312                  CSF2= CSF2 +(ETEP+ETAS+40.*WNIZN)/TMS
0313                  IF((MOD(NT,5).EQ.0).AND.(NT.NE.0)) SF1=CSF2 /(SO*EO*5.)
0314                  CSF1= CSF1 + SF2*DAVS
0315                   IF ((MOD(NT,5).EQ.0).AND.(NT.NE.0))  SF3=CSF1*DI5G
0316                   IF ((MOD(NT,5).EQ.0).AND.(NT.NE.0).AND.(SF3.LT.SF1*0.01)) SF3=
               XSQRT(SF1*SF3)
0317                  WGHT=SF1/SF3
0318                  SN=SO*DDEG*SF3*WGHT/ETV
0319                  NSW=ANSW+0.5
0320                  IF (SN.GT.ANSW)  NSW=SN +0.5
0321                  SWF=NSW/SN
0322                  NS=NSW*K2
0323                  SF=SWF
0324                  NMEW=WNMET +0.5
0325                  NEXW=WNEXC +0.5
0326                  W5VLE=W5VLE+ WVALUE*DAVS
0327                  CETEP=CETEP + ETEP*DAVS
0328                  CETAS=CETAS +ETAS*DAVS
0329                  CN5IZ=CN5IZ+WNIZN*DAVS
0330                  CNES=CNES+WNES*DAVS
0331                  CNAS=CNAS+WNAS*DAVS
0332                  CNMET=CNMET+WNMET*DAVS
0333                  CNEXC=CNEXC+WNEXC*DAVS
0334                  CESAVG=CESAVG+ ESAVG*DAVS
0335                  CEASG=CEASG+EASAVG*DAVS
0336                  CLOSS= CLOSS+(WNIZN-WNES)*DAVS/(TMS*SF3*WGHT)
0337                  WVLF1=W5VLE*DI5G
0338                  ALOSS=CLOSS*DI5G
0339                  ANSVG=CN5S*DI5G
0340                  ANIZVG=CN5IZ*DI5G
0341                  AETEP=CETEP/DTAVS
0342                  AETAS=CETAS/DTAVS
0343                  IF (ANIZVG.NE.0)  WVLE2=(EO*ANSVG-AETEP-AETAS)/ANIZVG
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0344              ANES=CNES/DTAVS
0345              ANAS=CNAS/DTAVS
0346              AESAVG=CESAVG*DI5G
0347              AEASG=CEASG*DI5G
0348              ANMET=CNMET*DI5G
0349              ANEXC=CNEXC*DI5G
0350              ANS=ANES+ ANAS -ANIZVG
0351              IF (ANS.LE.0.0)  ANS=NSW/SWF
0352              IF (ANIZVG.NE.0.0)  WVALUE= (SN*EO- AETEP-AETAS)/ANIZVG
0353              IF (WNIZN.NE.0.)  WVC=(ANS*EO -ETEP-ETAS)/WNIZN
0354              IF (NS.GE.1)  TMS=0.0
0355              NET=NES+NAS
0356              CALL  SOURCE(NS,NTP)
0357               IF (NET.GT.0)  CALL  FILHOL(NTP,NES, NAS)
0358           90 NIZNT= NIZNT +NIZW
0359              IF  (NUP .GT.0)  CALL  SEPROC(NTP, K3)
0360              IF (NONR.GT.0)  CALL  RRPROC(NTP,K3)
0361              NAST= NAST +NWS
                C  INTRODUCE THE SOURCE PARTICLES FOR THE NEXT CYCLE
                C EVERY FIFTH CYCLE RENORMALIZE NION AND OUTPUT QUANTITIES ARE PRINTED
                C RENORMALIZATION PROCESS OF NION
0362              AN5TP= 1.0/N5TP
0363              ANTP5=D5AVS/NTP5
0364              N5TPN=N5TP
0365              DO  16  M=1,JZ
0366              CNREZ(M)= CNREZ(M) + NREZ(M)*DAVS
0367           16 CEZ(M)= CEZ(M) + EZ(M)*DAVS
0368              DO  18  M=1,JZ
0369              FNREZ(M)=NREZ(M)*ANTPO
0370           18 EZ(M)= EZ(M)/ NREZ(M)
0371              SUMNE=0.0
0372              DO  193  M=1,JE
0373              SUMNE= SUMNE + NE(M)
0374              TNE(M)= TNE(M) + NE(M)/EDE(M)
0375          193 FNE(M)=NE(M)*ANTPO/EDE(M)
0376              EAV3=0.
0377              DO  1755  M=1, JE
0378              EAV3= EG(M)*FNE(M)*EDE(M) +EAV3
0379         1755 CNE(M)= TNE(M)*AN5TP
0380              CNION=CMUPOP*2.0*AIKT/SQRT(AKT*PI)
0381              ANION=0.0
0382              ANIO2=0.0
0383              DO  20  M=1,JE
0384              ANIO2= ANIO2 + FM1(EG(M),CNE(M))*EDE(M)
0385              ANION= ANION + FM1(EG(M),FNE(M))*EDE(M)
0386           20 CONTINUE
0387              DNION=ANION*CNION
0388              DNIO2=ANIO2*CNION
0389              CJD=ALOSS
0390              IF (ALOSS.LT.0.0)  CJD=0.0
0391              IF (ABS(CJD).GT.110.*SO)  CJD=110.*SO
0392              TNION=ABS(SO+CJD)/DNION
0393              TNIO2=ABS(SO+CJD)/DNIO2
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FORTRAN IV G LEVEL 18          MAIN          DATE = 72125          01/28/29

0394              TNIO2=SQRT(TNIO2)
0395              TNION=SQRT(TNION)
0396              CNIO2=CNIO2 + TNIO2*DAVS
0397              ANIOS=CNIO2*DISG
0398              WF=1.0
0399              IF (ANES+ANAS.NE.0.0)  WF=(ANIZVG+ANSVG)/(ANES+ANAS)
0400              IF  (MOD(NT,NPM).NE.0)  GO  TO  1790
0401              NION=ANIOS
0402              IF ((WF.GT.0.005).AND.(WF.LT. 200.)) NION=ANIOS*WF**NRF
0403           1790 CONTINUE
0404              DAVT=DAVG*ND
0405              ALPHA=WNIZN/(NTPW*DAVT)
0406              ANEAM=NICN*0.33333/DEN
0407           1785 FORMAT('0','ANION=',E13.4,3X,'DNION=',E13.4,3X,'TNION=',E13.4,3X,
                  X'ALPHA=',F12.5,4X,'LEAK=',E13.4,/)
0408              WRITE(6,1785)  ANION, DNIO2, TNIO2, ALPHA, ALOSS
0409              WRITE(6,171)  EO, PDPO, D, DETZ, DEG, NDPN
0410            171 FORMAT('1','GAS: HE',2X,'SOURCE ENERGY:',F5.0,3X,'PRESSURE:',F4.0,
                  X 'TORR',3X,'SLAB THICKNESS:',F4.1,' CM',' DX:',F4.1,' CM',4X,'DELT
                  X=',E12.5,3X,'#PROC=',I2,/ )
0411              WRITE(6,180) NT, TME, NS,NSW
0412            180 FORMAT(' ','NUMBER OF TIME CYCLES=',I6,3X,'TIME =', F12.5,' SEC',
                  1?X, 'GENERATED SOURCE PART =', I5,3X, 'WGTED # OF SOURCE PART.=',
                  1I5 )
0413              WRITE(6,1805) DAVT, DCEN1,EAVG,EWAVG, EAV3
0414           1805 FORMAT(' ','DAVG =',F12.5,3X, 'DCEN =',F12.5,3X,'OVERALL EAVG=',
                  1F10.5,3X,' WGTED EAVG=',F10.5,3X, 'EAVG CHECK=',F10.5,/)
0415              WRITE(6,191)
0416            191 FORMAT(' ', 1X,'NUMBER DISTRIBUTION',2X, 'FLUX DENSITY',4X,'AVERAGE
                  1E ENERGY',3X,'CUMULATED # DISTR',3X,'ENERGY INTERVAL',2X,'CUM FLUX
                  XDEN',4X,'#DEN-DEVIATION',/)
0417              CESUM=0.0
0418              DO  231  M=1, JE
0419              CESUM=CESUM + CNE(M)*EDE(M)
0420              IF (NE(M).GT.0)  DEAVG=EG(M)-EE(M)/NE(M)
0421              IF (NE(M).LE.0)  DEAVG=0.0
0422               IF (NE(M).EQ.0)  DNAVG=0.
0423              FNDV=CNE(M)-FNE(M)
0424               VFE=SQRT(EG(M))*ETV
0425              FLX1=FNE(M)=VFE
0426              FLX2=CNE(M)*VFE
0427              IF (NE(M).EQ.0)  GO  TO  281
0428              IF(((M.EQ.1).AND.(DEAVG.GT.0.0)).OR.((M.EQ.JE).AND.(DEAVG.LT.0.0))
                  X) DNAVG=-DEAVG*FNE(M)*0.5/EDE(M)
0429               IF ((DEAVG.LT.0.0).AND.((M+1).LE.JE)) DNAVG=-DEAVG*(FNE(M+1)-FNE(M
                  X))/(EG(M+1)-EG(M))
0430               IF ((DEAVG.GT.0.).AND.(M.GT.1)) DNAVG=DEAVG*(FNE(M)-FNE(M-1))/(EG(
                  XM)-EG(M-1))
0431            281 WRITE(6,182) M,FNE(M),FLX1,EG(M),CNE(M),EDE(M),FLX2 , DNAVG
0432            182 FORMAT(' ',I3,E12.5,5X,E12.4, 5X, F12.6,8X, E12.5,6X, F12.6,4X,E12
                  X.5,4X,E12.4)
0433              DET=DDEG/ETV
0434              WRITE(6,183) NTPP, NSTPN,NTPW ,DET, DAVGO, NCOL
```

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0435        183 FORMAT(' ',//,3X,'TOTAL # OF PARTICLES PROCESSED =',I5,5X,'CUMULAT
               1ED # OF PARTICLES =',I10,3X,'WGTED TOTL # OF PARTICLES=',F12.3,//,
               X' NEW QT=',E12.5,4X,'OLD QAVG=',F12.5,4X,'# OF COLLISIONS=',I5,///)
0436            WRITE(6,187)
0437        187 FORMAT(' '   ,1X, 'ZONE NUMBER', 5X, 'AVERAGE ENERGY',5X,'NUMBER O
               1F ELECTRONS',3X,'CUMULATIVE # DEN(Z)',3X,'CUMU. AVG ENERGY',3X,
               1'ZONE # DENSITY',/)
0438            DO 282  M=1, JZ
0439            ANZ=CNREZ(M)*ANSIP*0.15G
0440            PCZ=CEZ(M)/CNREZ(M)
0441        282 WRITE(6,184) M, EZ(M), NREZ(M), ANZ, PCZ,FNREZ(M)
0442        184 FORMAT(' ', 5X, I5, 5X, F14.6,8X,F14.6,  5X, F14.5, 7X,F14.6,7X,
               1F12.5)
0443            WRITE(6,185)  NION,WNIZN,NIZN, ANIZVG,WNES, NES,ANES, WNAS,NAS,
               XANAS, NTP, K1, K2, WF,BF
0444        185 FORMAT('0', 'NUMBER OF POSITIVE ION=',E14.6,//,' NUMBER OF IONIZAT
               1IONS OCCURED=',F9.3,5X,'ACTUAL #=',I5,3X,'CUMULATIVE AVG=' ,F10.3,
               X//,' # OF ESCAPED PARTICLES=',F9.3,5X,'ACTUAL#=',I5,3X,'CUMULATIVE
               X AVG=',F9.2,//,' # OF ABSORPED PARTIC=',E12.4,3X,'ACTUAL #=',I5,3X
               X,'CUMULATIVE AVG=',F9.2,//, ' TOTAL # OF PARTICLES IN THE NEW CYCL
               XE =',I5,//,' K1=',I2, 3X,'K2=',I2,     4X,' BALANCE   FACTOR WF=',
               XF10.5,3X,'BF2=', F10.5,/)
0445            WRITE(6,188) ED1, NPM, ND, KELC
0446        188 FORMAT(' ENERGY DIVIDING LINE FOR  RR PLAY E=',F10.4,4X,'EVERY',I2
               X,'TH CYCLE CHANGE N+',//,' TIME INTERVAL MULTIPLY FACTOR=',F9.4,
               X3X, 'ELASTIC XSEC / BY',I2,/)
0447            NDR=NDN-NDN/K3
0448            WRITE(6,186) NSO, NSW, ANSVG,NDR,WNSE,WNMET,ANMET,WNEXC,ANEXC,NUP,
               XWGHT
0449        186 FORMAT(' ',   ' SOURCE PARTICLES GENERATED OLD =',I10,//,
               1' SOURCE PARTICLES (WEIGHTED) IN THE NEW CYCLE =',I10,3X, 'CUMULAT
               XIVE AVG=',F10.3,//
               1,' # OF PARTICLES KILLED OFF IN RR PROC=',I10,//,
               I' # OF SUPER ELASTIC COLLISION=',F10.4,//,
               1                          ' # OF EXCITATIONS TO META STABLE LEVEL='
               X,F10.4, 3X, 'CUMULATIVE AVG=', F9.3,
               1                          //,' # OF EXCITATIONS TO OTHER LEVELS=',F10.4,
               X4X, 'CUMULATIVE AVG=',F9.2,//,' # OF PARTICLES CROSS OVER TO HIGH
               XENERGY REGION NUP=',I5,4X,'OVERALL WT=',E12.4,/)
0450            WRITE(6,195)  EF, EDP, PDPO ,SF1, SF2, SF3
0451        195 FORMAT (' E-FIELD=', F9.2,'V/CM', 4X,'E/P=',F9.2,4X,'P/PO =',F7.1,
               X3X, 'SF1=', E12.4,3X, 'SF2=',E12.4,3X, 'SF3=', E12.4,/)
0452            WRIT=(6,170) SO,WVC,SWEO,WVALUE,WVLE1, WVLE2,ESAVG, AESAVG,EASAVG,
               XAEASG
0453        170 FORMAT(' SOURCE RATE =',E11.3,' PER SEC',4X,'W-VALUE(LOCAL  )=',
               XF10.3, 3X,'SOURCE RED.FACT=',F13.4,//,' W-VALUE=',
               XF10.3,4X,'CUM AVG WV1=',F9.3,3X,'CUM AVG WV2=',F9.3,
               1      //,' AVERAGE ENERGY OF ESCAPED PARTICLES=',F12.5,3X,'CUMULAT
               XIVE AVG=',F11.4,//,' AVERAGE ENERGY OF ABSORPED PARTICLES=',F12.5,
               X3X, 'CUMULATIVE AVG=',F11.4,/ )
0454            CKENE=SUMNE*ANTPO
0455            WRITE(6,189)CKENE, CESUM, TNION, TNIO2
0456        189 FORMAT(' ','THE SN # CHECK =',F12.4,3X,'THE CN # CHECK=',F12.4,//,
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                    1''CALCULATED N+ USE P=',E14.6,3X,'CALC. N+ USE CN =',E14.6,3X, 'AR
                    XTIF CN+=',E14.6,//)
0457                IF ((MOD(NT,3).NE.0).OR.(MOD(NT,10).EQ.0)) GO TO 3
0458                WRITE(9) EAVG, DAVG, TME, NTW, NT, NTP, NION,DDEG, NSW,SWF, E, U
0459                WRITE(9) Z, WT ,ANIOS, SF3
0460                ENDFILE 9
0461                REWIND 9
0462              3 CONTINUE
0463                IF (MOD(NT,10).NE.0) GO TO 4
0464                WRITE(10) EAVG, DAVG, TME, NTW, NT, NTP, NION, DDEG, NSW,SWF, E, U
0465                WRITE(10) Z, WT ,ANIOS, SF3
0466                ENDFILE 10
0467                REWIND 10
0468              4 CONTINUE
0469                IF (MOD(NT,NCUM).NE.0) GO TO 6666
0470                N5TP=0
0471                NTP5=0
0472                D5AVS=0.0
0473                NAST=0
0474                NIZNT=0
0475                W5VLE=0.0
0476                CLOSS=0.0
0477                CSF1=0.0
0478                CNIO2=0.0
0479                CN5IZ=0.0
0480                CN5S=0.0
0481                CNMET=0.0
0482                CNEXC=0.0
0483                CESAVG=0.0
0484                CEASG=0.0
0485                DO 54 M=1,JZ
0486                CNREZ(M)=0.0
0487             54 CEZ(M)=0.0
0488                DO 55 M=1,JE
0489                TNE(M)=0.
0490             55 CNE(M)=0.0
0491                IF (MOD(NT,10).NE.0) GO TO 6666
0492                DTAVS=0.0
0493                CETEP=0.0
0494                CETAS=0.0
0495                CNES=0.0
0496                CNAS=0.0
0497             6666 CONTINUE
0498                NT= NT + 1
0499                DO 56 M=1,500
0500                DIZN(M)=0.0
0501                IRR(M)=0
0502                IES(M)=0
0503             56 IAS(M)=0
0504                DO 51 N=1,50
0505                WSE(N)=0.0
0506             51 ESE(N)=0.0
0507                I=1
```

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      C  REINITIALIZE THE OUTPUT QUANTITIES
0508                DO  52  M=1, JE
0509                EE(M)=0.
0510             52 NE(M)= 0.0
0511                DO  53  M=1,JZ
0512                NREZ(M)= 0.0
0513                EZ(M)=0.0
0514                DO  53  N=1,JE
0515                EKZ(N,M)=0.0
0516             53 NEZ(N,M)=0.0
0517                NIZN=0
0518                NOZN=0
0519                NIN=0
0520                NES=0
0521                NSE=0
0522                NCOL=0
0523                NAS=0
0524                DTOT=0.0
0525                NMET=0
0526                NEXC=0
0527                WNAS=0.0
0528                WNSF=0.0
0529                WNES=0.0
0530                WNIZN=0.0
0531                WNMET=0.0
0532                WNEXC=0.0
0533                ETAS=0.0
0534                ETEP=0.0
0535                ETOT=0.0
0536                NUP=0
0537                NDN=0
0538                NDNR=0
0539                INIV=INIV+ 1100
0540                CALL    REINZ(INIV)
0541                WRITE(6,72)
0542                IF (NT.LE.NTC)  GO  TO  7777
0543             9999 STOP
0544                DEBUG  SUBCHK
0545                END
```

VITA

Benjamin Shaw-hu Wang was born in Inner Mongolia, China, on March 25, 1937. He is the son of Mr. C. H. Wang, the former Chinese Army General now the Congressman of the Republic of China. He received the B.S. degree in Electrical Engineering from the National Taiwan University of Taipei, Taiwan, China in 1960, he then served as an ensign in Chinese Naval Academy for one and a half years. He came to the United States in September, 1962 and enrolled in the University of Missouri at Rolla, Missouri. After he received the M.S. degree in Electrical Engineering in 1964, he joined the Westinghouse Research Laboratories and served as a research engineer for three and a half years.

In September 1967, he came to the University of Illinois at Urbana-Champaign to undertake studies for a Ph.D. in Computer Science Department. He has been a research assistant and teaching assistant in the Department of Computer Science and a research assistant in the Nuclear Engineering Program. He is the member of Kappa Mu Epsilon and Pi Mu Epsilon the two national honor societies of mathematics.

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A Monte Carlo simulation model for radiation induced plasmas with nonlinear properties has been developed, which employs a piecewise linearized predict-correct iterative scheme to resolve nonlinear characteristics. Several variance reduction techniques have been developed and incorporated into the model which include the antithetic variates technique. The model has been applied to the determination of electron energy distribution functions in a noble gas plasma created by α-particle irradiation. The model can be applied to other types of complex plasma problems with nonlinear properties.

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